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Plenary

50 years in thermal analysis with biological and medical applications JTACC Scientific Excellence Award 2025

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Keywords: microcalorimetry, DSC, muscle proteins/fibers, blood plasma

In this presentation I sum up our research activity from this field performed in the last 50 years. I will focus on the next main points: basic research in muscle heat production and the different intermediate states of ATP hydrolysis cycle in muscle proteins and muscle fibers, R&D activities to develop and test different dairy products and TA applications in some surgical and diagnostic procedure. Our initial research concerned the building a sensitive microcalorimeter [1] to investigate the cross striated muscle heat production in different type of muscle contraction [2]. the investigation of thermal stability of main muscle proteins when their basic unfolding characteristics were clarified. Our first paper discussed the conformational changes in bovine heart myosin studied by EPR and DSC. It was followed by the skeletal G and F-actin, and we extended the thermal stability investigation from protein solution to the myosin myofibrils, checking the effect of nucleotides in different ATP hydrolysis steps. We have got further help for the interpretation of these states from the studies of cooperative stabilization of actin filaments by phalloidin and jasplaklinolide [3] as well as from the BeF_x treated actin filament experiments. After it we tested the higher organization of muscle proteins, the muscle fibers. At that time became possible to stabilize the different intermediate states of ATP hydrolysis up to the time of DSC measurement. At very first we checked the effect of oxygen free radicals in myosin head. It was continued with muscle fibers using different P_i analogues (V_i, AlF_x and BeF_x) and non-hydrolysable ATP analogue (AMP.PNP). Our biggest success was to prove at very first that the AM.ADP and rigor states differ from each other not only from biochemical but internal molecular dynamic point of view too [4,5]. With our R&D cooperation a cold spreadable butter [6] was successfully developed. We were partners in the development of Ca-enriched cheese [7], in its spreadable form too as well as in the development and testing of different dairy products using probiotic cultures [8]. Our TA activity covers a wide range of medical applications. We could follow by TA the different abnormalities of human skeletal muscle in leg [9]. We have found a good agreement between the DSC scans and different stages of degeneration of human vertebral discs too. We could judge the goodness/applicability of different suture techniques on tracheal cartilage in primary airway reconstruction. TA was successfully used in the characterization of different self-expandable stents implantation in the oesophagus treatment [10]. We could monitor the effect of shoulder arthroscopic capsullography by DSC. We investigated the thermal consequences of tendon and ligament rupture of leg. We have joined those groups [11] who try to use DSC in the diagnosis of different diseases from blood plasma e.g. in case of breast cancer, melanoma [12] and psoriasis [13] as well as from red blood cells in different stages of diabetes [14].

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Challenges with carbon allotropes

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Keywords: carbon materials, carbon fibers, carbon nanotubes, CCVD

Carbon-based materials are used in many fields of science and technology. Carbon materials have played an important role for humans since prehistoric times; for example, charcoal as a heat source and adsorbent, natural graphite powder in pencils, carbon black in black ink. However, the 20th century brought a significant breakthrough in the discovery and application of new forms of carbon. It is impossible to judge which form of carbon is of the greatest technological importance, but it may be worth exploring the similarities between carbon fibers and carbon nanotubes in a lecture.

Carbon fibers are produced from different precursors by different processes, and as a result they have different nanotextures and structures. Both the precursor and the production method have influence on the nanostructure of carbon fiber; however, the heat treatment temperature is crucial for the structure and thus for controlling the properties. Nowadays, carbon fibers are widely used (in reinforced plastics and other composites), although it is not possible to list all applications here.

Over the past three decades, carbon nanotubes have been a constant focus of attention in the scientific community due to their extraordinary physical, chemical, thermal and electrical properties. Within the family of CNTs, vertically aligned carbon nanotubes can play an important role in electrical, mechanical development and as additives for composites.

To our knowledge, the only way to produce vertically aligned carbon nanotubes ("CNT forests") is using the catalytic chemical vapor deposition (CCVD) technique. The first important step in the synthesis is the construction of a thin catalyst layer on a suitable substrate, which is pre-coated with an insulating layer. At the beginning of the CCVD synthesis, the thin layer is transformed into nano-sized catalyst particles by heat treatment and a reductive atmosphere. These will then seed the growth of carbon nanotubes in the presence of a carbon source feed, which will form an ordered structure after reaching a critical length. During CCVD, a number of parameters (reaction time, reaction temperature, gas etc.) influence the growth, allowing the properties of the CNT forests to be fabricated to be under control. The role of the support layer, the transformation of the catalyst layer in the presence of hydrogen gas and the growth mechanism of carbon nanotubes were confirmed by thermodynamic considerations.

Compared with the technological applicability of carbon fibers of the micron scale, the use of nanometer carbon nanotubes raises a number of challenges for both researchers and engineers. There are many steps from the atomic level to the final product, including the design and optimization of multi-scale systems, which involve regular feedback at all levels of the design.

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Thermal analysis methods in thermal energy storage applications

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Keywords: Thermal Energy Storage, sensitive, latent, thermochemical, thermal analysis methods, renewable energy

Thermal Energy Storage (TES) is an emerging and crucial technology for addressing global energy challenges. It is extremely relevant in the context of the ongoing transition to renewable energy sources. Renewable energies are intermittent by nature, the sun does not always shine or the wind blows, and it is a great challenge to accommodate consumption and production. Finding cost-effective, global and reliable storage solutions is essential to increase reliance on these renewable sources. TES offers a solution to mitigate power outages and increase energy access, contributing to the decarbonization of energy systems, reducing reliance on fossil fuels and supporting the shift toward sustainable, low-emission energy sources, which is vital in the fight against climate change. TES involves materials that can store heat and then release it when needed, making it an effective solution for balancing energy supply and demand. Thermal energy can be stored as sensitive, latent and thermochemical. Research is focused on improving the efficiency, capacity, and cost-effectiveness of TES technologies, which are critical for energy systems transitioning to more sustainable sources.

Thermal Analysis methods play a crucial role in thermal energy storage (TES) research by providing essential insights into the thermal properties, behaviour, and performance of materials used in TES systems. These methods provide information about how materials absorb, store, and release heat, which is fundamental for optimizing TES technologies. Thus, they are used for optimization of materials and cyclic conditions. In this lecture an overview of our experience in this field will be provided.

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Microscale combustion calorimetry used in thermal hazards research

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Keywords: microscale combustion calorimetry, flammability, fire safety

In fire safety science, Microscale Combustion Calorimetry (MCC) is a novel experimental tool for assessing the heat release characteristics and flame retardant behaviour of materials. MCC is a rapid flammability analysis instrument based on the oxygen consumption principle, and using milligram-scale specimens under controlled pyrolysis. By measuring the heat released during the thermal decomposition of materials, MCC provides critical data on the heat release rate, helping researchers understand the fire hazards of materials. It offers advantages such as minimal sample usage, rapid testing, making it widely applicable in the development of flame-retardant materials, fire risk assessment, and the optimization of fire resistance in building materials. The application of MCC provides essential experimental evidence for fire safety science, contributing to the development of more effective fire prevention and response strategies. This presentation covers the structure and testing procedure of MCC, the application limitations of MCC, a correlation study between MCC and bench-scale instruments, as well as several use cases of MCC.

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Invited

Solid state thermoanalytical characterization of drugs and pharmaceuticals by thermoanalytical techniques

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Keywords: physicochemical characterization, DSC, mass spectrometry, API, polymorphism, thermal stability, amorphous drugs, drug–excipient compatibility.

The solid-state characterization of active pharmaceutical ingredients (APIs) and drug formulations is a critical component of modern pharmaceutical development, directly influencing stability, bioavailability, manufacturability, and regulatory compliance. Thermoanalytical techniques, particularly Differential Scanning Calorimetry (DSC), Thermogravimetric Analysis (TGA), Modulated DSC (MDSC), and Hot-Stage Microscopy (HSM), offer powerful and complementary tools for probing the thermal behavior of pharmaceutical solids. This presentation focuses on the application of these thermal techniques to evaluate polymorphism, crystallinity, amorphous content, thermal stability, and drug–excipient compatibility. Case studies will be discussed to demonstrate the use of DSC and MDSC in detecting polymorphic transitions, eutectic formation, and glass transition temperatures in poorly water-soluble drugs. TGA will be highlighted for its role in assessing moisture content, thermal degradation kinetics, and quantifying volatile components. HSM, used in conjunction with DSC, provides visual insight into phase transitions and melting behavior. A special emphasis is placed on preformulation studies where solid-state screening and compatibility testing via thermal methods guide the rational selection of excipients and processing conditions. Further, the utility of advanced techniques such as hyphenated methods (TGA-FTIR, TGA-MS) will be outlined for comprehensive decomposition profiling. Overall, thermoanalytical characterization ensures the development of thermally stable and robust pharmaceutical products by establishing a deep understanding of solid-state properties. The integration of these methods into the drug development pipeline not only expedites formulation optimization but also strengthens regulatory documentation in line with ICH Q6A guidelines.

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The true role of phase change materials in thermal management and energy efficiency

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Keywords: phase change materials, latent heat, thermal performance, evaluation method, buildings

Phase change materials (PCMs) are substances that absorb or release heat when they undergo a phase transition. Phase change materials are extensively used in thermal energy storage systems, buildings, electronic thermal management, photovoltaic panels, and other applications due to their ability to store and release significant amounts of latent heat at nearly constant temperatures, as well as their availability across a broad range of phase change temperatures. This growing interest is driven by their potential to enhance energy efficiency, improve thermal management, and contribute to sustainable building practices. In buildings, PCMs can be integrated into external walls, ceilings, floors, and glazing systems, resulting in energy savings, effective energy demand shifting, stabilized indoor temperatures, and enhanced thermal comfort. The use of PCMs in both industrial and residential settings is anticipated to grow, increasing their significance in the advancement of next-generation energy systems. The versatility of PCMs, with their ability to be tailored to specific temperature ranges, makes them suitable for various climates and building types. On the other hand, given that the performance of PCMs is influenced by several factors, such as phase change temperature, latent heat capacity, thermophysical properties, and climatic conditions, a proper index or evaluation method should be employed to accurately quantify the effectiveness of PCMs. In this talk, various evaluation methods will be addressed, the thermal performance of PCM in buildings will be assessed along with the conventional techniques, and several case study-based evaluations will be presented to highlight the advantages and disadvantages of each method/parameter, enabling a clearer interpretation. The talk will attempt to offer insights into how PCMs can contribute to the development of more efficient and sustainable thermal management solutions in building designs.

Off-line evolved gas analysis with the coupled system TGA/DSC–IST16–GC/MS: case studies

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Keywords: TGA/DSC–IST16–GC/MS, thermal degradation, evolved gas analysis, fire safety, hyphenated techniques

Thermogravimetric analysis (TGA) in combination with a mass spectrometry (MS) and/or an infrared spectrometry (FTIR) is most commonly used to determine the type and amount of gas produced as a decomposition product from a variety of materials. TGA, coupled with gas chromatography (GC) and mass spectrometry, is better suited for analysing complex gas mixtures and the decomposition products that occur simultaneously in low concentrations and often overlap.

Our Mettler Toledo TGA/DSC–IST16–GC/MS instrument provides insight into a sample with its combination of a gas chromatograph (GC) and an MS. The GC separates the collected gases so that simultaneously collected substances can be better identified by the MS detector. One system includes a heated storage interface (IST) that can store up to 16 gas fractions collected at different temperatures during a TGA experiment. It enables the emission profile of selected evolved compounds as a function of thermogravimetric decomposition temperature [1].

In this contribution, we present this new approach to explain the successful solution of puzzles with results obtained using only one spectroscopic technique. For example, we used TGA–MS and complementary DSC techniques in combination with microscopic observations to explain the mechanism of action of the intumescent coating, the efficiency and the compatibility with our substrate, wood. A very important part of the MS analysis remained unanswered and relates to the toxicity of the smoke during combustion in terms of the formation of gases with mass peak $m/z = 78$, which could be benzene. Only with the help of chromatographic separation and identification by GC/MS were we able to confirm the identity of this peak with the TGA/DSC–IST16–GC/MS instrument from Mettler Toledo.

The addition of phase change materials (PCMs) in the form of encapsulated PCM paraffins to building materials changes their specific heat capacity and optimises energy consumption in buildings. As PCM paraffins are flammable, TGA-MS and TGA-GC/MS were combined to check the thermal stability interval, analyse the gases released and investigate their potential toxicity in the event of a fire.

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Impact of various trivalent metal ions on thermal, structural, morphological and magnetic properties of zinc ferrite

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Keywords: zinc ferrite, trivalent metal ions, silica matrix, doping, annealing, magnetic behavior

Zinc ferrites doped with various metal ions exhibit good chemical stability, wear resistance, good mechanical hardness, high coercivity, moderate saturation magnetization, high Curie temperature, high magneto-crystalline anisotropy, good electrical insulation, high electrical resistivity, and are attractive candidates for data storage and magneto-optical devices, memories, sensors, color imaging, ferrofluids, and favorable candidates for targeted drug delivery, magnetic resonance imaging, tissue repair, biosensors and hyperthermia [1-6]. The sol-gel route has the advantages of simplicity, flexibility, low cost, good control over the structure and properties, and production of nanosized ferrites with reliable and reproducible physical properties [1-4]. The ability to tailor the structural, magnetic, and electrical properties by selecting the synthesis parameters and the doping ion allows the widespread use of ferrites. This work presents the effect of trivalent metal (La^{3+}, Cr^{3+} and Bi^{3+}) ions doping and annealing temperature (400, 800, and 1200 ^{o}C) on the thermal, structural, morphological and magnetic properties of $ZnFe_2O_4$ embedded SiO_2 matrix synthesized by sol–gel method. The thermal behavior of the reactants during the synthesis process revealed the formation of metallic succinates up to 200 °C and their decomposition into metal oxides, which further react to form the ferrites. Fourier-transform infrared spectroscopy confirmed the embedding of undoped and doped $ZnFe_2O_4$ nanoparticles in the SiO_2 matrix at all annealing temperatures. X-ray diffraction (XRD) showed that at low temperature annealing resulted in poorly crystalline ferrites, while high temperature annealing directed to highly crystalline ferrites accompanied by secondary phases of the SiO_2 matrix. Crystallite size, lattice parameter and porosity are proportional to the dopant content. The atomic force microscopy (AFM) images revealed spherical ferrite particles covered by an amorphous phase, with particle size, powder surface area, and coating thickness depending on the doping ion and annealing temperature. The structural parameters calculated by XRD and AFM, as well as the magnetic parameters were contingent on the doping ion and annealing temperature. The evolution of saturation magnetization (M_S), coercivity and magnetic anisotropy as a function of the crystallite sizes was studied by vibrating sample magnetometry (VSM) technique. The *Ms* was influenced by the particle size and crystallinity only for nanocomposites annealed at 800 and 1200 °C, when the magnetic domains started to form and to be larger than the critical particle size. The nanocomposites exhibited ferrimagnetic behavior, close to the superparamagnetic limit. A strong correlation was found between the particle morphology and the magnetic properties of the nanocomposites. The hysteresis loops showed a direct relationship between the annealing temperature and saturation magnetization at constant coercive field.

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Some factors affecting the results of kinetic analysis

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Keywords: kinetic analysis, thermal decomposition

Kinetic analysis of the thermally stimulated processes, i.e., the processes that are initiated by a change in temperature can have either a practical or theoretical purpose. A major practical purpose of the kinetic analysis is the prediction of process rates and material lifetimes while its major theoretical purpose is interpretation of experimentally determined kinetic triplets [1]. In both cases, the reliability, correctness and consistency of the calculated kinetic parameters is expected and implied. However, even a cursory review of the literature reveals the existence of differences in the results of kinetic analysis of thermal decomposition processes for the particular material. What causes these inconsistencies in the kinetic results? Are they due to the specific material properties during thermal decomposition or to the applied kinetic computational methods? What is the role of the researchers in the kinetic calculations? Some examples of the kinetic analysis of the thermal decomposition of polymers that may give indications of a possible answers and stimulate discussion will be presented.

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Thermal stability and decomposition mechanism of nitrocellulose

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Keywords: energetic materials, spontaneous decomposition, thermal safety, heat flow calorimetry

Nitrocellulose (NC), a nitric acid ester compound containing an ONO_2 functional group, is widely utilized as a raw material in explosives, lacquers, and celluloid products. Although NC has a wide range of industrial applications, it is highly unstable and prone to spontaneous decomposition even at low temperatures. The accumulation of decomposition heat can lead to spontaneous ignition, posing a risk of severe accidental explosions[1]. While the spontaneous decomposition of NC has been investigated for many years, recent incidents seem to have renewed interest in understanding its reaction mechanisms and improving safety measures based on scientific evidence. Previous studies have shown that reactive species such as O_2 and H_2O in the surrounding environment, as well as NO_2 and HNO_3 generated from NC itself, accelerate its exothermic decomposition[2]. However, the detailed reaction mechanisms remain to be fully elucidated. This study aims to clarify the role of these reactive species in the spontaneous decomposition of NC and to contribute to a more comprehensive understanding of its decomposition pathways. To achieve this, the authors performed heat flow calorimetry on NC at heating rates of 0.05 K/min or lower in air and N_2 atmospheres with the addition of NO_2, H_2O, and HNO_3. This experimental approach enabled the evaluation of the effects of different reactive species on the decomposition behavior of NC. The experimental results revealed distinct effects of each additive on NC decomposition. Specifically, NO_2 lowered the decomposition temperature of NC only in air. In an N_2 atmosphere, the decomposition behavior remained unchanged regardless of the presence or absence of an excessive amount of NO_2 (5,000 ppm), suggesting that the effect of NO_2 on NC decomposition depends on the presence of O_2. In contrast, both H_2O and HNO_3 lowered the decomposition temperature in both air and N_2 atmospheres, with HNO_3 exhibiting a more pronounced impact than H_2O. These findings suggest that while NO_2 alone cannot sustain radical chain reactions without O_2, the formation of HNO_3 during NC decomposition and its conversion from NO_2 in the presence of H_2O may be crucial for maintaining these reactions. Furthermore, our quantum chemistry studies, based on first-principles calculations, propose a decomposition mechanism for an NC model compound (NC_m) that includes the generation pathways of NO_2 and HNO_3, as well as their interactions with NC_m in the presence of O_2. The experimentally observed thermal behaviors in this study align with the proposed mechanism, supporting its validity.

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Hydration of biomolecules in the solid state: insights from isothermal and temperature scanning calorimetry

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Keywords: water sorption, hydration, differential scanning calorimetry, glass transition, sorption calorimetry

The primary industrial interest in water-biomolecule interactions in the solid state lies in their role in pharmaceutical formulations, particularly for biologics [1]. This topic also holds fundamental importance, as it allows for the investigations of concepts related to thermal behaviour of amorphous substances. In particular, carbohydrates used as excipients in pharmaceutical formulations serve as convenient objects for studying glass transition and water sorption behaviours.

Glass transition is a fundamental property of amorphous systems, which, when properly analysed, provides valuable insights into their physical characteristics. The simplest approach for describing the glass transition is the so-called "minimal model" [2], which based on two parameters offers a basic description of thermal properties in the glass transition region. Although too simplified for comprehensive understanding of the phenomenon, it is adequate for the description of glass transition in samples with certain thermal histories [3]. Thermal history is generally a crucial factor to control for correct interpretation of calorimetry and water sorption data on biomolecules in the solid state [3,4].

In glassy carbohydrates, water activity deviates from the expected equilibrium values, often leading to sorption-desorption hysteresis. The partial molar enthalpy of mixing of water (often referred to as hydration enthalpy) is negative in the glassy state and shows relatively complex profiles when studied by water sorption calorimetry [5,6]. This behaviour was recently explained based on the glass transition properties of the components [7]. To further develop this approach, we derived an expression for water activity in glassy materials, where the deviation from the equilibrium activity values is related to heat capacity changes of the components of the system [8].

Acknowledgments
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Compressing experiences of resolution trials into ternary equilibrium melting phase diagrams by DSC and powder XRD

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Keywords: chirality, optical resolution**,** crystalline racemates, enantiomers, diastereomeric salts, resolving agents

Formation and fractionated crystallization of diastereomeric salts or co-crystals is one of the most frequently applied and probably one of the simplest methods of optical resolution on binary mixtures of enantiomeric molecules with mirror image [1, pp. 39-41]. In general, binary mixtures of crystals, based on the extent of their miscibility in solid phase, can be classified into three fundamental types, such as a) a physical mixture, i.e. conglomerate of crystals showing eutectic relation (if components are fully immiscibility in crystalline state); b) forming (at least) one new common crystalline addition compound in a definite stoichiometric ratio, which is usually in eutectic relation with the parent crystalline phases (as case of partial miscibility of components in solid phase); c) solid solution (components which are fully miscible in any ratio in crystalline state). These cases for solid molecular pairs can be characterized and represented by means of binary (melting point) phase diagrams build upon series of differential scanning calorimetric (DSC) measurements, even for fusion of racemic binary compositions [1, p.32], [2]. Liquidus curve of melting phase diagrams can be modelled by simplified Schröder - van Laar or Prigogin-Defay equations in case of eutectic crystal conglomerates or racemic compounds of enantiomers, respectively [1, pp. 46-47, 88-91], [2] using only the individually measured melting points ($T_{m,i}$ in K) and molar enthalpy values of fusion (ΔH^f_i, J/mol) of pure crystalline enantiomeric components.

When applying a resolving agent, inevitable a third component occurs in the racemic resolution system, ternary fusion phase diagrams are also needed to describe and represent detailed complexity of the whole system, beside the pairwisely obtainable binary ones [3]. A triangular fusion phase diagram of the two mirror enantiomers together with the chosen resolving agent usually composed of joining several three-component fusion phase (sub) diagrams of three-component (eutectic) immiscible crystalline phases [4], as a result of occurrence of one, two or more crystalline diastereomeric phases in the resolution system.

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Dedicated to Prof. Dr. Elemér Fogassy on the occasion of his 90th birthday. Many Happy Returns of the Day!

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Catalytic hydrodeoxygenation of bio-oil produced from co-pyrolysis of biomass and plastic waste

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Keywords: biomass, plastic, co-pyrolysis, bio-oil, red-mud, upgardation

The rising energy demand and the decreasing availability of fossil fuels have driven the pursuit of renewable fuel sources from biomass and plastic waste [1]. However, biofuel production faces challenges due to the high free fatty acid content in waste lipids [2]. To improve fuel quality, oxygen removal is essential. This study explores the catalytic hydrodeoxygenation of bio-oil derived from the co-pyrolysis of *Mesua ferrea* L. (Nahar, a non-edible oilseed) and PET plastic. Operating parameters, including temperature and biomass-to-plastic ratio, were optimized, revealing a maximum bio-yield of 35 wt% at 600 °C with a 2:1 biomass-to-plastic ratio. Qualitative analysis of the co-pyrolyzed oil showed that fatty and carboxylic acids (~55%) were the dominant components, necessitating further upgrading for potential applications. In the upgrading process, red mud (RM), an alkaline waste from alumina production via the Bayer process [3], was used as a support material for mono-metallic (Ni) and bi-metallic (Ni-Co) catalysts. These catalysts were characterized using BET, FESEM-EDX, FETEM, XRD, ICP-MS, and XPS. They were then applied in the hydrodeoxygenation (HDO) of co-pyrolytic oil, with the Ni-Co/RM catalyst achieving the highest organic liquid yield (72%) while minimizing coke formation and maximizing hydrocarbon yield (80%). Using mono- and bi-metallic catalysts at a reaction temperature of 300 °C, the HDO process effectively reduced the acid content of raw bio-oil (~55%) while significantly enhancing hydrocarbon yield (80%). The primary reaction pathways observed were hydrodeoxygenation (HDO) and decarboxylation (DCO).

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Immersion calorimetry in adsorption science: bridging thermodynamics and surface

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Keywords: immersion calorimetry, adsorption thermodynamics, surface interactions, porous materials

Immersion calorimetry is a powerful and precise technique that offers fundamental insights into adsorption thermodynamics and solid-liquid interactions. This talk will explore its principles in depth, emphasizing how immersion enthalpy measurements can uncover critical information regarding adsorption mechanisms, energetic heterogeneity, and the physicochemical nature of surfaces.

The discussion will begin with an overview of the theoretical foundations and instrumentation involved in immersion calorimetry, emphasizing its role in characterizing porous materials. By quantifying the heat released or absorbed during immersion, this technique enables researchers to differentiate between textural and chemical contributions to adsorption. Furthermore, it provides valuable data on surface polarity, wettability, and the strength of solid-liquid interactions, which are essential for understanding adsorption behavior in various systems.

Experimental methodologies will be examined, focusing on sample preparation, probe liquid selection, and interpreting calorimetric signals. Case studies will illustrate their application in environmental remediation, catalysis, and advanced materials, demonstrating utility in evaluating adsorption efficiency, energy distributions, and material stability.

Finally, recent advancements and future perspectives in immersion calorimetry will be addressed, including developments in high-sensitivity microcalorimeters and innovative experimental approaches. As adsorption science evolves, this technique remains a vital link between thermodynamics and surface chemistry, facilitating the design of more efficient adsorbents for sustainable applications.

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Different approaches towards the optimization of $BaCeO_3$-based composite protonic conductors

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Keywords: ceramic protonic conductors, composite materials, co-doping, spark plasma sintering (SPS), hot pressing (HP), electrical conductivity, chemical stability

ABO_3-type compounds represent a group of ceramic proton conductors considered for use in many electronic and electrochemical devices, such as fuel cells, high-temperature electrolysers or gas sensors. Barium cerium oxide, $BaCeO_3$, crystallizing in perovskite structure exhibits relatively the highest protonic conductivity in this group of ionic conductors. Many strategies have been proposed to improve the electrical properties and chemical stability of $BaCeO_3$-based materials, such as the formation of solid solutions (e.g. with $BaZrO_3$), forcing the non-stoichiometry in the cation sublattice by changing the Ba/Ce ratio, doping in the B position with trivalent atoms, as Y, Yb, etc., or by modification of the grain boundaries by introducing an additional phase and formation of composites. Also, different materials preparation methods and uncommon sintering methods (SPS, HP) were also used to prepare materials with desired properties, among others the highest possible ionic (protonic) conductivity and high chemical resistance in an environment containing water vapor and CO_2.

In this work we present our results concerning different approaches towards the optimization of $BaCeO_3$-based materials. We have applied a modification using different dopants: isovalent (such as Zr) and aliovalent (such as Y and Yb), also including co-doping strategy. We have tested the possibility of formation of composites by introduction of various modifier phases based on the Ba-Ce-Y-Si-P-O glassy-crystalline system into the $BaCe_{0.9}Y_{0.1}O_3$ host material using various preparation methods: mechanical homogenization or impregnation in solution. We have also employed and compared different sintering methods: free sintering of pellets, Spark Plasma Sintering (SPS) or Hot Pressing (HP) under controlled conditions.

The obtained materials were characterized and examined using X-ray diffraction (XRD) and scanning electron microscopy (SEM) techniques. Electrical properties were determined using Electrochemical Impedance Spectroscopy (EIS) as a function of gas atmosphere and temperature. Chemical stability was evaluated using the DSC-TG method. Based on the analysis of the obtained results, the influence of the chemical composition and preparation method on the phase composition, structure, microstructure, electrical properties and chemical stability of the prepared materials was determined and discussed. The improvement of selected properties for some systems investigated indicates that the use of particular modifications can be a promising way towards the $BaCeO_3$ based protonic conductors with improved properties.

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Thermal properties of “all-bio” polymeric materials reinforced by natural (nano)fibres

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Keywords: all-bio polymeric materials, thermal properties, natural (nano)fibres

Current research trends in the area of new materials include the design and preparation of polymer composites taking into account the need to reduce the consumption of non-renewable resources and environmental protection requirements, including ease of recycling. The solutions sought include "all-bio" systems that use polymers synthesized from monomers obtained from renewable raw materials, such as biopolyamides or biopolyolefins, as well as biofillers. Among the latter, an important place is occupied by cellulose, a common natural polymer which, when used as an additive, also with nanometric dimensions, can beneficially improve the properties of the polymer matrix. However, when manufacturing polymer composites modified with natural fillers, their thermal resistance is insufficient and degradation occurs under melt processing conditions. The selection of the matrix-fiber system plays an important role, also to ensure proper adhesion of the components and to prevent (or minimize) the effects of agglomeration during classic processing (extrusion, injection) or using additive technologies. In this context, the appropriate method of obtaining and modifying cellulose becomes crucial. Applied methods of modifying cellulose nanofibers (CNF), including e.g. esterification with acid anhydrides, carboxymethylation or silanization lead to increased compatibility with the polymer matrix and improved thermal stability to enable high-temperature processing. Importantly, for industrial applications, it is required to increase the scale of production of bio(nano)fillers and ensure high quality/repeatability of the characteristics of biomaterials.

The lecture will focus on the thermal properties of biopolymer composites modified with natural fibers and the prospects for further development of this promising group of polymeric materials..

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Thermal conversion and characterization of tanned leather

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Keywords: leather, thermogravimetry/mass spectrometry, pyrolysis, tanning agent, charcoal

In today's world, the effective management of leather waste is becoming increasingly vital. Tanned leather wastes are mostly generated in the automobile and light industry. However, the conversion of leather waste into value-added products shows significant challenges due to the presence of tanning agents, finishes, and various additives. Thermochemical processes, including slow and fast pyrolysis, offer promising avenues for transforming leather waste into valuable materials. For example, nitrogen-enriched charcoal can be used as a catalyst support for transition metals utilized in fuel cells or as catalysts in chemical reactions. The transition metals supported by nitrogen-rich charcoal has the potential to replace the expensive precious metal catalysts that are currently in use, paving the way for more cost-effective and sustainable solutions.

In this work, carbonaceous residues from tanned leathers were prepared at temperatures of 400, 500, and 700 °C for one hour in a laboratory-scale tube furnace under a nitrogen atmosphere. Variously tanned bovine hides were applied in this project: vegetable-tanned leather using quebracho extract, chromium III-tanned leather, and mixed mineral-vegetable tanned leather using aluminium salt and myrobalan extract. The yield of charcoal decreased as the temperature of the thermal treatment of tanned leathers increased. Furthermore, the solid yield from the mixed and vegetable-tanned leathers was higher compared to that derived from chromium-tanned leather indicating that vegetable tannins significantly enhance the char formation. The nitrogen content of both the raw materials and the resulting carbonaceous products was measured using the Dumas method. It was found that the charcoal produced from chromium-tanned leather had the highest nitrogen content. Consequently, charcoal samples with elevated metal content (chromium or aluminium) may lead to the development of new and cost-effective catalytic materials.

Thermoanalytical methods have been applied to characterize the leather and charcoal samples. The analytical techniques such as thermogravimetry/mass spectrometry (TG/MS) and pyrolysis-gas chromatography/mass spectrometry (Py-GC/MS) are highly effective in assessing the thermal stability and the composition of the raw materials and the charcoals. The composition of the volatile decomposition products was also determined, since utilizing the energy content of these byproducts could improve the cost-effectiveness of the industrial process.

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Thermophysical characterization of functionalized metallic particles during phase change processes

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Keywords: molecular dynamics simulations, nanoencapsulated phase change materials, heat capacity, latent heat, density

There has been increased interest in the use of functionalized metallic particles in additive manufacturing (AM) processes. By utilizing these types of functionalized metallic powders in AM processes, enhanced mechanical properties have been observed in the AM-processed parts, including improved density, increased hardness, and increased tensile/yield strength. However, a fundamental understanding of the underlying physics that are present during the thermal processes of AM has yet to be developed. In this talk, results obtained from molecular dynamics simulations will be presented that provide insight into the characteristics of thermophysical properties of coated metallic particles during phase change processes. Particle structure, melt temperature, and heat capacity are analysed for their response to particle coating/functionalization. A comparison of results obtained from these molecular dynamic simulations and experimental investigations is also addressed. Finally, this talk will conclude with a discussion on how these responses could potentially influence the development of process parameter sets that are used in the additive manufacturing of metallic parts using these functionalized metallic particles.

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Electrical and thermal safety characteristics of aged lithium-ion batteries

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Keywords: internal material degradation, aging mechanisms, electrical parameter analysis, characterization analysis, thermal analysis

The mature development of lithium-ion batteries (LIBs) has led to their widespread applications in various devices. However, safety concerns after prolonged LIBs usage remain a distinct issue. After multiple cycles, **internal material degradation** and reduced thermal stability will occur, with different usage conditions leading to varying degrees of aging, potentially resulting in irreversible thermal runaway. This study investigates three aging conditions: Normal charge (NC), Rapid discharge (RD), and Overcharge/discharge (OC). Over a limited period, 50 cycles were conducted to analyze their **aging mechanisms** and effects. Various analytical techniques were employed, including **electrical parameter analysis**, such as direct current internal resistance (DCIR), electrochemical impedance spectroscopy (EIS), and incremental capacity analysis (ICA); **characterization analysis**, such as field emission-scanning electron microscopy (FE-SEM) and X-ray diffraction (XRD) analysis; and **thermal analysis** using differential scanning calorimetry (DSC) and an accelerating rate calorimeter (ARC). Finally, the study explores the correlation between electrical parameters and the consequences of thermal runaway.

The results indicated that, under the OC conditions, DCIR exhibited the highest increase (29.49 mΩ), and the state of health (SOH) dropped to 94.41%. EIS results showed a semicircle appeared in the OC condition. ICA analysis revealed the most intense chemical reactions near 4.2 V and new peaks emerging in the low-voltage region. FE-SEM analysis indicated increased cathode crystallites under OC conditions and fractured anode surfaces under RD conditions. XRD results confirmed that aging did not alter the primary material composition. Thermal analysis results showed that the exothermic heat release decreased after aging, and the apparent exothermic onset temperature (T_{onset}) increased. Under OC conditions, the cathode's heat release dropped to 97.7 J/g, and T_{onset} increased to 229.27 °C. Under adiabatic conditions, 12 key parameters were analyzed, revealing that the maximum cell center temperature (T_{cell}) reached 894.07 °C for NC, while RD and OC conditions resulted in 752.31 and 719.50 °C, respectively. As aging progressed, the maximum pressure (P_{max}) under OC conditions reached 8.07 barG, indicating that aging conditions affect internal materials, leading to changes in thermal stability and the consequences of thermal runaway.

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Various degrees of conversion in thermoanalytical kinetics

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Keywords: degree of conversion, thermoanalytical kinetics, general rate equation, elementary reaction, complex process

Kinetics of condensed-phase processes are routinely studied by methods based on the general rate equation. It is demonstrated here that, for the kinetic analysis, two degrees of conversion should be discriminated: (i) the degree of conversion used in classical kinetics, α_{kin}, conventionally defined as the reacted amount of a reactant normalized to its initial amount; (ii) the thermoanalytical degree of conversion, α, defined as the thermoanalytical effect observed at temperature T (or at time t for isothermal measurements) divided by the total thermoanalytical effect [1].

For elementary reactions, $\alpha_{kin} = \alpha$ so that the general rate equation is a true rate equation describing the mechanism of the reaction. For complex processes, α_{kin} and α differ considerably in general; they are equivalent for some special cases only. In this case, the general rate equation represents the single-step approximation [2]. The values of α thus describe the kinetics of heat exchange (for DSC) or mass loss (for TG) and so do the kinetic parameters obtained from the treatment of experimental data. Even though no mechanistic conclusions should be drawn from such kinetic parameters, they still enable us to model the kinetics of complex processes from the point of view of the quantity measured, i.e., the heat evolution/consumption or mass loss [1].

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Thermal analysis and multifunctional applications of advanced ZnO-based materials obtained by various chemical methods

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Keywords: ZnO, thermal analysis, sensors, piezoelectric

In the present work the synthesis, thermal behaviour, and multifunctional applications of advanced ZnO-based materials obtained using sol-gel, hydrothermal and microwave-assisted sol-gel methods are presented. The mentioned synthesis techniques offer control over the purity, crystallinity, and morphology of the resulted nanomaterials. The research focuses on doped ZnO materials, including ZnO-SnO_2 composites and ZnO doped with Mn, V, and Cu, targeting applications in sensing, piezoelectric devices, photocatalysis, and nanofluids.

The influence of dopants and synthesis methods on the thermal stability and structural properties is thoroughly examined. Thermal analysis, supported by complementary techniques such as infrared spectroscopy (IR) and X-ray diffraction (XRD), revealed critical correlations between synthesis conditions, dopant incorporation, and the thermal behaviour of the resulted materials.

Results show that ZnO-SnO_2 composites provide enhanced sensitivity for gas sensing, Mn and V-doped ZnO films exhibit strong piezoelectric potential, while Mn-doped ZnO powders demonstrate high photocatalytic efficiency under solar light, and Cu-doped ZnO nanostructures for nanofluids present improved thermal stability and antibacterial performance.

These insights contribute to the tailored development of ZnO-based materials for advanced technological applications.

Lithium ion battery fire behavior and preventions

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Lithium ion batteries are essential in a broad range of strategic industries such as automotive, power grid, aerospace and consumer electronics. However, lithium ion battery thermal runaway arises from a series of undesirable side reactions accompanied by an uncontrolled temperature ascending, sometimes catastrophically accompanied by fire and explosion, which has impeded their further development. In this report, the thermal runaway mechanism is revealed from the heat generation, side reactions decoupling, thermodynamics, and thermal abuse test. Subsequently, the fire prevention strategies are proposed from the intrinsic safety, process safety, fire safety perspectives, of which the safe electrolyte, thermal management methods, fault diagnosis and fire suppression are considered to enable safe lithium ion battery. In the future, we appeal closer collaborations between the academia and industry to drive integration, improvements, harmonization and application of lithium ion safety across fields.

Application of thermal analysis in the synthesis and characterization of clay mineral-based nanostructures and photocatalysts

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Keywords: kaolinite, halloysite, intercalation, exfoliation, composite, nanostructure, photocatalysts

Clay minerals are abundant, cheap, natural and widely applied industrial resources. Members of the kaolinite-group, such as kaolinite and hallyosite, are 1:1 type, layered phylloaluminosilicates, constituted by Si^{4+}-centered tetrahedral (T) and Al^{3+}-centered octahedral (O) layers forming TO layers, which are held together by hydrogen-bonds, resulting in a typical, layered structure. Their intrinsic surface properties and morphology can be artificially modified by various methods. Nanoscrolls with increased surface area and tubular morphology can be synthesized via a multi-step intercalation and exfoliation processes [1,2]. The use of clay minerals in the remediation of environmental elements are promising, especially their use as adsorbents and photocatalysts [3]. One of the most remarkable achievements of clay mineral research has been the proof of the photochemical activity of kaolinite [4,5]. The exfoliated nanoscrolls showed a unique potential to be photocatalysts [6]. Surface-deposition of photocataltically active components (such as transition metal oxides or graphitic-like materials) could result in composite systems, resulting in a more favorable dispersity, a possible sensitivization towards visible-light adsorption and a significant increase of photocatalytic activity.

This talk will give an overview of our current results of 1:1 type phylloaluminosilicate based nanostructure and photocatalyst research by cascade intercalation, nanostructure synthesis via exfoliation and composites formation, and their potential application in photoinduced catalysis and environmental remediation. Kaolins and halloysites with various origins, mineral composition and crystallinity, along with synthetic kaolinite, were utilized. Clay-mineral based composites having different transition-metal oxides (e.g. TiO_2, ZnO, CuO, NiO) or non-metallic photocatalysts (e.g. graphitic carbon nitride) were synthesized and investigated for the photocatalytic removal of various aqueous pollutants. Thermal treatment in the synthesis phase of composite catalysts could be critical, as controlled thermal dehydroxillation of kaolinite and halloysite might result in defect sites with reduced coordination environments (^{V}Al, ^{IV}Al), which could significantly improve catalytic activity [7]. Structural elucidation methods were applied for sample characterization, including vibrational spectroscopy (FTIR-ATR, Raman spectroscopy), X-ray diffraction (XRD), transmission electron microscopy (TEM) with energy-dispersive X-ray (EDX), porosity measurements by liquid nitrogen adsorption (BET/BJH-SSA), Mössbauer and ^{27}Al MAS NMR spectroscopy, X-Ray adsorption (XAS) along with thermal analysis (TG/DTG/DTA-DSC). Photocatalytic activity were determined by using UV-Vis and fluorescence spectroscopy.

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Recent developments in accessories at ta instruments increasing analysis flexibility

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Keywords: TGA, sealed pans, JavaScript object notation

For over 60 years, TA Instruments has been at the forefront of materials characterization, delivering innovative thermal analysis, rheology, microcalorimetry, and mechanical testing solutions to laboratories worldwide. Renowned for precision engineering and scientific excellence, TA Instruments continues to evolve with the needs of modern research and quality control. Among their recent advancements are **self-punch pans**, which streamline sample preparation and improve consistency in thermal analysis workflows. Additionally, the introduction of **JSON export functionality** in data files enhances data accessibility and integration, enabling seamless interoperability with modern data analysis pipelines and laboratory information systems. These innovations reflect TA Instruments' ongoing commitment to empowering scientists with tools that are not only accurate and reliable but also efficient and future-ready.

Revolutionary DSC 5+ — Sets new standard in research with Differential Scanning Calorimetry

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Material science and market need to develop new materials is fast growing chemistry field and therefore also Thermal analysis have become important field for research. Differential Scanning Calorimetry is one of techniques which provide us relevant results.

Mettler-Toledo developed new modern Differential Scanning Calorimeter DSC 5+ to measure, detect, evaluate and interpretate thermal events when material is expose to different temperature programs. Instrument allow to heat or cool samples with different heating rates or keep samples at isothermal conditions.

New ceramic sensor which is built in DSC 5+ holds two technologies: technology based on Heat Flux or Power Compensation principle. We can easy detect very small effects with HeatFlux technology where are 136 Thermocouples built in[1] or with use of Power Compensation technology with 2 heaters and Pt sensors which keep temperature on a sample and reference side equal we are capable to determine cp values with an error less than 1%[2].

This presentation will highlight technical details of new DSC 5+ and provide some applications.

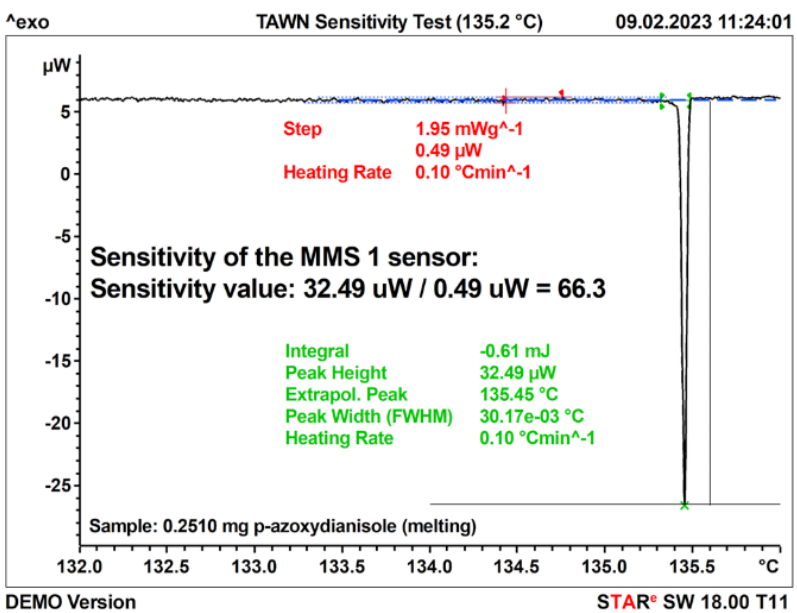

Figure 1: TAWN sensitivity of new DSC 5+.[1]

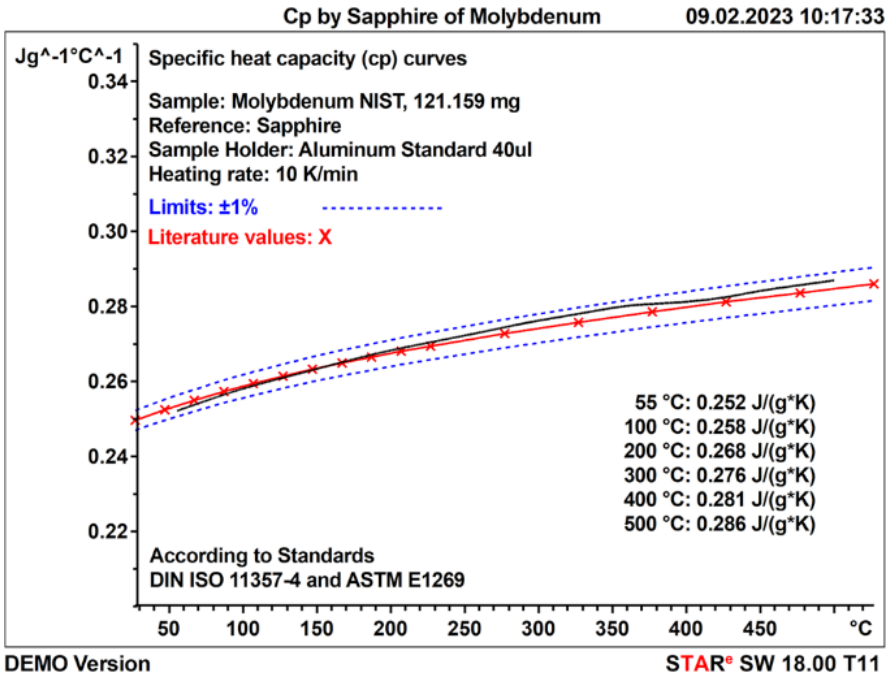

Figure 2: cp determination of Molybdenum with new DSC 5+.[2]

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1. An Advanced Heat Flux DSC Operated in the Power Compensation Mode, Jürgen E.K. Schawe, Book of Abstracts of the 25th Braunschweiger Kalorimetrietage 2023, page 69
2. Wie man die Messleistung eines dynamischen Differenzkalorimeters qualifizieren kann, Matthias Wagner, Werkstoffe 4/2023, page 14/15

Hyphenation and visualization techniques in thermal analysis and their applications

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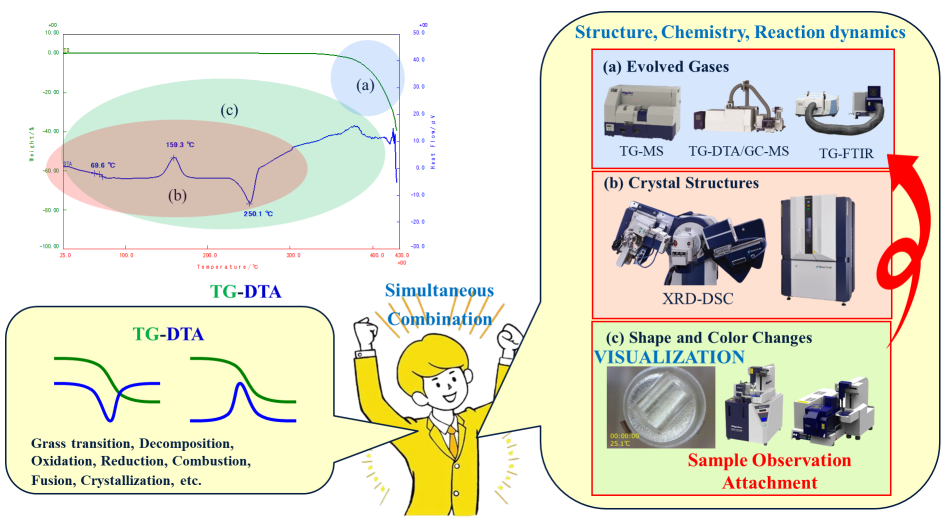
Keywords: TG-MS, TG-FTIR, XRD-DSC, sample observation, visualization

Thermal analysis can be widely applied to understand thermal properties and chemical changes on the "macromolecular level". For example, simultaneous thermal analysis (STA or TG-DTA/DSC) is not only a powerful option for evaluating the thermal properties of materials, but also allows for more detailed analysis of the gas products evolved by the thermal decomposition of materials, thanks to the realization of simultaneous measurement systems combining STA with mass spectrometry (TG-MS) [1-2] or Fourier transform infrared spectroscopy (TG-FTIR). Similarly, simultaneous XRD-DSC [3], a technique that combines X-ray diffraction (XRD) and differential scanning calorimetry (DSC), is a technique that simultaneously measures the thermal changes of the solid phase by DSC and the changes in the crystalline state by XRD. It is a powerful analytical tool that can continuously monitor the changes in crystalline materials accompanying phase transitions such as polymorphic transformation, dehydration, crystallization, and solidification.



Another major innovative technology until recently has been "visualization analysis". Sample observation analysis that integrates the optical microscope with the thermal analysers to observe the change in the materials during thermal measurements does not only reveal the visible changes directly in sample shape, size, colour and other properties, but also is

significantly useful to help the interpretation of an accurate chemical or physical transformation. The thermal changes in the sample status can be displayed in real time and because the optical visual images can be automatically linked with the thermal characteristic data from the thermal analysers as well as the temperatures, the playback analysis can be carried out just by clicking the data curves. By introducing sample observation function, it was visually revealed that the intermediate crystalline phase exists during the crystallization processes from the crystal liquid. To demonstrate the effectiveness of the unique hyphenated and/or visualized thermal analysis methods developed in recent years, application results for several materials will be presented

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Oral Presentations

T01: Bio sciences, including food, soil, textile, wood

Rumen fermentation of date seed fractions: chemical, structural, and thermal modifications for potential food applications

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Keywords: date seeds, fermentation, holocellulose, rumen

Date seeds, a by-product of date fruit, are an underutilized lignocellulosic polymer that accumulates in nature. In this study, date seeds were processed through grinding, defatting (with petroleum ether), and de-lignin (with ethanol) to produce a control fraction (H-C). Rumen liquor from cows was then used to treat the H-C, resulting in two fractions: the residual (HCR) and supernatant (HCS). The chemical, structural, and thermal properties of these fractions were analyzed. Significant changes were observed in the chemical composition of the HCR fraction, with cellulose, protein, and fat content increasing to 25.0, 18.0, and 6.0 g/100g, respectively, compared to the control (47.0, 6.0, and 0.4 g/100g). The solubility of the HCR (15.0 g/L) and HCS (58.0 g/L) fractions increased significantly compared to the control (4.0 g/L). The thermal analysis showed distinct glass transitions, with the HCR fraction showing a single transition (G1: 154°C) and the HCS fraction displaying two (G1: 38°C and G2: 89°C), indicating greater compositional heterogeneity in the latter. The HCR fraction also exhibited a higher solid melting temperature (182°C), indicating lower degradability. Surface morphology and crystallinity changes confirmed that rumen treatment altered the structural integrity of the fractions. Further research is needed to assess the safety and sensory properties of these fractions for potential food applications.

Reactive chlorinated triazine phytate ester for flame retardant modification of silk fabric: flame retardancy and mode of action

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Keywords: flame retardancy, thermal degradation, mechanism, phytic acid, covalent grafting

Phytic acid, a natural and eco-friendly bio-based material, has attracted increasing attention in flame retardancy research [1]. Previous studies have demonstrated its effectiveness in textile flame-retardant finishing; however, its poor washing durability limits practical applications, as it primarily interacts with silk fabrics via electrostatic forces. In contrast, reactive dyes form strong covalent bonds with fibers, ensuring excellent washing fastness. Inspired by X-type reactive dyes, this study synthesized a novel reactive flame retardant, Chlorinated Triazine Phytate Ester (CTPE), by combining phytic acid, ethanolamine, and cyanuric chloride, mimicking the molecular structure of X-type reactive dyes. A low-temperature impregnation method was successfully employed to covalently graft CTPE onto silk fibers. As shown in **Fig. 1**, the modified silk fabrics exhibited excellent flame-retardant performance, with a limiting oxygen index (LOI) of 33.7% and a reduced char length of 8.7 cm. Even after 20 washing cycles, the fabric retained its self-extinguishing properties, confirming the durability of the flame-retardant effect. Compared to untreated silk, the modified fabric exhibited a substantial decrease in total heat release (THR) and total smoke production (TSP) by 23.2% and 77%, respectively. Thermogravimetric analysis (TGA) revealed that the modified silk had a lower thermal degradation rate under a nitrogen atmosphere, with a residual char yield of 41.2% at 700 °C, significantly higher than that of untreated silk. Fourier transform infrared (FTIR) analysis of the char residue identified distinct absorption peaks at 990 cm^{-1} and 1100 cm^{-1}, corresponding to the stretching vibrations of P-O-P, P-O-C, and P=O groups [2]. Raman spectroscopy further confirmed a lower I_D/I_G ratio in the char residue of modified silk compared to untreated silk, indicating a higher degree of graphitization and enhanced thermal stability. These findings suggest that phosphorus-containing derivatives promoted the dehydration and carbonization of silk fibers, enhancing residue graphitization and forming a stable carbonaceous layer. This protective barrier effectively isolated oxygen and combustible components, thereby suppressing further combustion. In summary, CTPE provides an effective and durable flame-retardant effect on silk fabrics, primarily through its condensed-phase action.

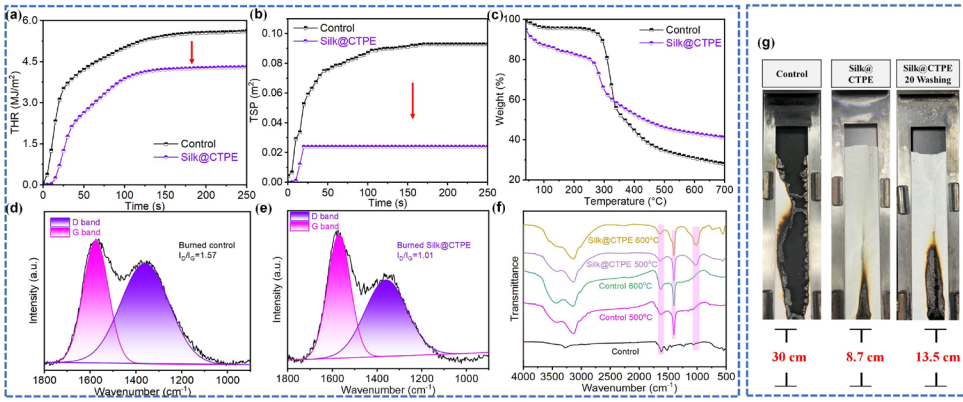

Fig. 1. The THR (a), TSP (b), TG (c), Raman (e), and residual FTIR spectra (f), and the vertical burning photos (g) of the modified silk fabrics.

Acknowledgments

This study was funded by the Key Research and Development Program of Suzhou (SYC2022017), the National Natural Science Foundation of China (22408247).

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Assessing the affinity of bioactive isolates from different *in vitro* digested coffee fraction extracts by binding to PPAR-γ using isothermal titration calorimetry and docking simulation

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Keywords: PPAR-γ, keywords here, separated, with commas

Peroxisome proliferator-activated receptor-γ (PPAR-γ) is a hormone mainly responsible for gene expression involved in fats and carbohydrates metabolism. This results in increased levels of insulin sensitivity, contributing to maintaining glucose homeostasis [1, 2]. It has three types of gamma isoforms (γ1, γ2 and γ3) of which the PPARγ2 protein is 30 amino acids shorter at the nitrogen terminus [3]. The activation of PPAR-γ by their ligands induces the expression of proteins, such as lipoprotein lipase. This reduces inflammation and thereby controls fatty acid metabolism, regulating fatty acid transport and adipogenesis [4]. Synthetic PPAR-γ agonists, such as thiazolidinediones, are used in antidiabetic therapy. The use of this substance for a long time causes negative effects on the human body, among others swelling and inflammation. That is why, natural ligands are sought and we used in our research bioactive compounds contained in coffee. To assess the possible degree of PPAR-γ activation and to select the most stable complexes of compounds contained in coffee subjected to *in vitro* digestion with the PPAR-γ receptor and to determine the type of bonds, we used isothermal titration calorimetry (ITC) and performed molecular docking simulation.

ITC analysis of the interactions of fractions isolated from coffee extracts showed an increase in the binding constant by about 10% after gastric digestion compared to the value before digestion. The interactions of digested fractions of coffee extracts with PPAR-γ showed an exothermic energetic effect, regardless of the digestion stage. It gradually increased as digestion progressed.In the initial phase of digestion, the reaction enthalpy decreased from the range of -8.70− -2.40 kJ/mol for the caffeine fraction from green Arabica and Robusta to the range of -8.16− -0.63 kJ/mol for the fraction of dichlorogenic acids isolated from green Robusta coffee and monochlorogenic acids from lightly roasted Arabica. In the presence of probiotic bacteria in the further part of the digestion, a renewed increase in the negative enthalpy of the reaction was observed, which did not occur in parallel *in vitro* digestion tests without bacteria. However, the presence of selected strains of probiotic bacteria resulted in a reduced affinity of the components of the coffee extract fraction to the receptor compared to samples digested without bacteria. This work was supported by the National Center of Science [grant numbers UMO-2018/29/N/NZ9/01160].

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Investigation on flame retardancy and mechanism of the coated PA6 fabrics by using phosphorylated bio-derivative

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Keywords: flame retardancy, thermal degradation, anti-dripping, quenching effect, durability

Polyamide 6 (PA6) fiber is renowned for its exceptional wear and abrasion resistance, high tenacity and toughness, excellent fatigue behavior, and good resilience [1]. Consequently, PA6 fiber materials have found applications across various industries, including military, electronics, aerospace, and transportation sectors [2]. However, PA6 fabrics are highly susceptible to ignition, and during combustion, flaming droplets can ignite nearby flammable materials, triggering a catastrophic chain reaction. Therefore, enhancing the flame-retardant properties of PA6 fabrics is of paramount importance. In this study, a novel phosphorylated p-coumaric acid bio-derivative, designated DOPO-pCA, was synthesized using bio-based p-coumaric acid and DOPO. This compound was then applied to PA6 fabrics to improve their flame retardancy. Given the inherently low reactivity of PA6 fabrics, a self-polymerization strategy was employed to enhance the washing durability of the coated PA6 fabrics. A comprehensive investigation was conducted to evaluate the FR properties of the coated PA6 fabrics, with a particular focus on flame retardancy, washing durability, combustion behavior, and the underlying flame-retardant mechanisms. As shown in **Fig. 1**, the coated PA6 fabrics exhibited excellent self-extinguishing and anti-dripping capabilities. After functional coating treatment, the limiting oxygen index (LOI) of the coated PA6 fabric increased from 23.5% to 31.0%, while the damaged length decreased from 18.2 cm to 12.3 cm. Fourier-transform infrared (FTIR) analysis revealed characteristic peaks for phosphorus-containing compounds at 1530, 1360, 1320, and 1120 cm^{-1}, corresponding to P-CAr, P=O, and P-O bonds, respectively, with an additional peak for the Ph-O bond at 1290 cm^{-1}. These findings confirmed the presence of phosphorus-oxygen and phenoxy free radicals. These active species could effectively capture H· and ·OH radicals during combustion, thereby quenching the flame reaction and enhancing flame retardancy. This enhanced quenching effect resulted in a 32.4% reduction in the average effective heat of combustion (av-EHC). Furthermore, the peak heat release rate (pHRR) and total heat release (THR) were reduced by 30.7% and 22.4%, respectively. Due to the self-polymerization and inherent reactivity of DOPO-pCA, the flame-retardant performance of the coated PA6 fabric showed only slight degradation after 30 washing cycles.

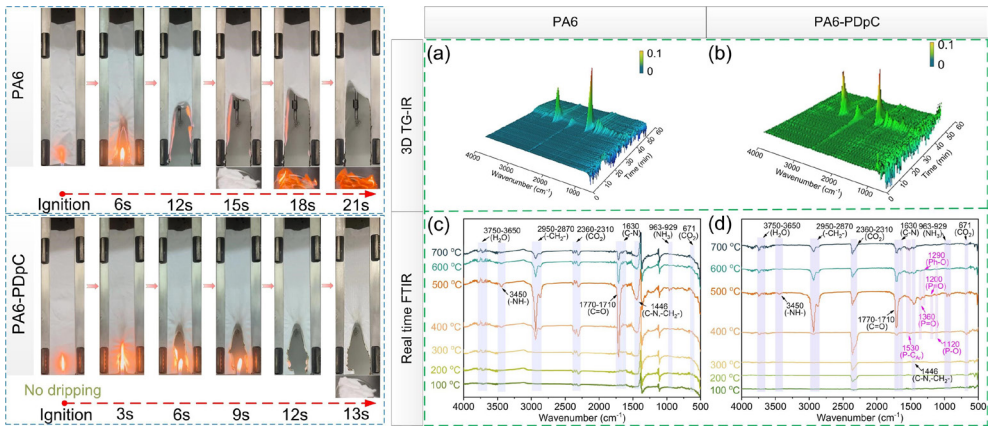

Fig. 1. The combustion behavior of PA6 fabrics during vertical burning test, and 3D TG-IR curves of PA6 (a) and coated PA6 (b), detailed IR curves of PA6 (c) and treated PA6 (d) under nitrogen.

Acknowledgments

The present work was funded by the Key Research and Development Program of Suzhou (SYC2022017) and the National Natural Science Foundation of China (22408247).

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State diagram of freeze-dried coriander leaves by measuring and modelling freezing curve, maximal-freeze-concentration condition, glass and Solids-melting lines

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Keywords: coriander, glass transition, food stability, freezing curve, solids melting-line, maximal-freeze-concentration

State diagram is an advanced stability map to determine different states or phases of a food as a function of temperature and solids content, and it could be used to determine the physical and chemical stability during processing, storage and even during consumption, digestion and absorption in stomach. In this study, a state diagram for coriander leaves was developed by measuring glass line, freezing curve, maximal-freeze-concentration condition, glass and solids-melting curves. The solids content was varied from 0.05 to 0.99 g/g coriander leaves. Freezing point decreased with the increase of solids content, while glass transition and solids-melting decreased with the decrease of solids content. Freezing curve was modelled by Chen's equation based on Clausius-Clapeyron equation and glass line was modelled by Rahman-Gordon-Taylor equation. The characteristic ultimate maximal-freeze-concentration conditions $(T_m)_u$ (i.e. end temperature of freezing) and $(T_g)_u$ [i.e. end glass transition at $(T_m)_u$] were measured as −30.9 °C and −24.4 °C, respectively. The characteristic maximal-freeze-concentration solids content (i.e. X_S was determined as 0.70 g/g coriander leaves by drawing a vertical line passing through $(T_m)_u$ in the state diagram. Therefore, un-freezable moisture content was considered as 0.30 g/g coriander leaves. Solids-melting was modelled by Flory-Huggins's equation, and solids-water interaction parameter was estimated as 0.69 indicating very high binding of water with solids matrix. Thirteen micro-regions were mapped in the state diagram and could be used to determine stability of coriander leaves when temperature and water content varied during processing and storage. In the future work, specific physical or chemical changes need to be measured in these micro-regions and need to determine their kinetics in each micro-region.

Flame retardant behaviour and smoke/heat suppression of organic-inorganic intumescent polyelectrolyte complexes on fabrics

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Keywords: intumescent coatings, polyelectrolyte complexes, flame retardant, fabrics, coatings

Flame-retardant coatings have demonstrated effective fire protection and many applications for various materials. The development of innovative flame-retardant coatings with the advantages of improved sustainability, ease of processing, high efficiency as well as simple-to-scale-up assembly has attracted increasing attention. Herein, micro/nano-structured ceramizable organic-inorganic hybrid coatings were designed inspired by nacre structure consisting of polymers (polyethyleneimine (PEI), gelatin, cellulose nanofibrils) and nanoparticles (montmorillonite, laponite, graphene oxide) as ceramic precursors to form polymer-layered nanocomposites. The coatings can be assembled onto the surface of substrates by a simple two or several-step process at low temperature. Upon a flame, the coatings can form a micro intumescent noncombustible char layer that can act as an oxygen barrier and heat shield for substrates. The coated fabrics exhibited rapid self-extinguishing performance and heat/smoke inhibition ability without significant mechanical strength decreasing. The novel application of sustainable biobased components in this works provides a new effective strategy for the development of a desirable performance portfolio and fire-safe materials.

Acknowledgments
This work is supported by the State Key Laboratory of Wuhan Science and Technology Bureau Supported Special Fund (2022023988065193) and the Key Laboratory of Textile Fiber and Products (Ministry of Education), (Wuhan Textile University) (Fzxw2024010).

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T02: Calorimetry

Thermal characterization of biobased alternatives to paraffin wax for candle formulation

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Keywords: biobased materials, candle, combustion, thermal analysis

The candle industry primarily relies on paraffin wax [1], a petroleum-derived material that participates to the mechanical properties and combustion properties of candles due to its high melting point and enthalpy. However, its fossil-based origin raises environmental concerns. As sustainability gains importance, biobased alternatives are being explored [2]. In particular, rice bran wax (RBW) and hydrogenated rapeseed oil (HRO) appear to be promising candidates to paraffin wax substitution owing to their thermal properties or/and combustion behaviour.

Differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) were used to compare the thermal properties of two biobased raw materials (RBW and HRO) with that of a semi-refined paraffin (SRP). DSC results revealed higher melting temperatures for RBW and HRO compared to that of SRP, while RBW had the lowest melting enthalpy among the three materials. TGA showed that SRP decomposed in a single step, whereas biobased alternatives exhibited a multi-step degradation, indicating a more complex thermal stability.

Combustion properties i.e. burning time, mass consumption, and burning rate of the corresponding candles were then evaluated. Combustion tests demonstrated that SRP based candles exhibited the longest burning time with the highest mass consumption and combustion rate. HRO followed, while RBW had difficulty burning, with less than 5% of consumed material. Although candles formulated with semi-refined paraffin presented higher combustion performance, candles with HRO remained in acceptable quality criteria.

Thus, HRO appeared as a promising alternative, whereas RBW may require formulation adjustments or blending strategies to improve its combustion efficiency. These results also highlight that DSC could be an interesting method to discriminate raw materials, though it has to be combined with others to optimize biobased formulations and to achieve performance comparable to conventional paraffin candles.

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Modular peltier-based isothermal battery-calorimeter

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Keywords: calorimetry, batteries, ibc

Calorimetric tests on batteries are commonplace. Using classical differential dynamic calorimetry methods, the materials of a battery, such as anode and cathode material, can be easily identified and examined with regard to their thermal stability. Accelerating rate calorimetry can also be used to investigate extreme conditions, short circuits and mechanical penetration. A modular isothermal battery calorimeter has now been developed in collaboration with the Physikalisch-Technische Bundesanstalt and Linseis Messgeräte GmbH. The background to this is that the influences of environmental conditions and their impact on the performance of battery cells can be investigated using an easy-to-use measuring device. Not only individual cells, but also several cells can be examined. This allows to investigate the influence of the stability of several cells as well as their housing. In addition to the sample, the user can adjust the format of the measuring cell between 80 mm x 80 mm and 300 mm x 300 mm as well as the cooling for the desired temperature range of the tests. The voltage source of the battery in the form of a laboratory power supply unit or a specific charger can also be used here in order to carry out tests that are as realistic as possible. With this new setup, we want to demonstrate and discuss possibilities for testing batteries in different areas of application for quality testing and under different environmental conditions as well as their ageing with manageable effort.

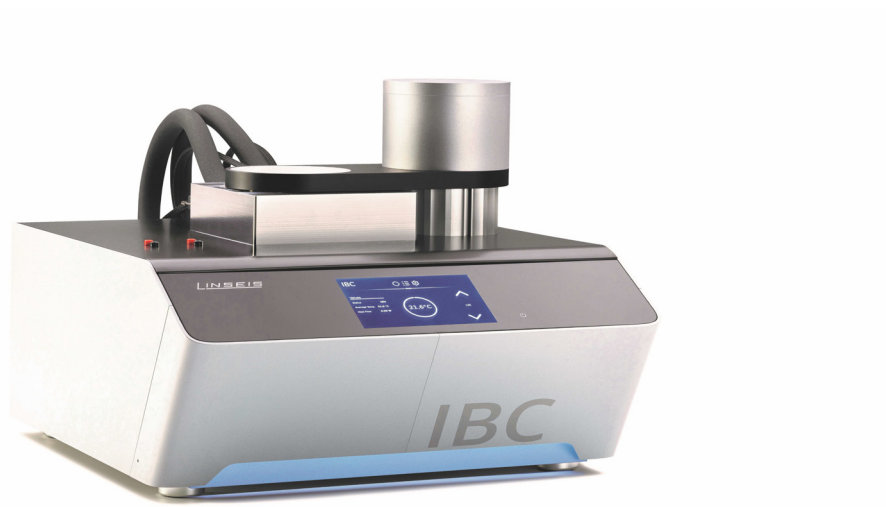

Figure 1 Isothermal Battery Calorimeter IBC L91 80

Acknowledgments
We would like to thank Stefan Sarge and the entire Physikalisch-Technische Bundesanstalt for the many years of good cooperation and their services to science. Their outstanding achievements are a core element of many metrological developments and methods.

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Impact of electrolyte and combustible gases on the control characteristics of lithium-ion batteries before thermal runaway

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Keywords: energy security, secondary battery chemistries, liquid electrolyte, passive safety mechanism, combustible gases

In response to contemporary energy demand issues, energy security becomes the most urgent challenge. Problems like energy depletion, environmental pollution, and global warming forced people to seek innovative solutions to alleviate reliance on fossil fuels. The remarkable advantages of high energy density and long cycle life set lithium-ion batteries apart from other well-known secondary battery chemistries. Because of the poor thermal stability of the liquid electrolyte in lithium-ion batteries, it was prone to internal decomposition and gas generation. When the gas accumulated to a certain pressure, it triggered the battery's passive safety mechanism, causing it to enter an irreversible state. During this process, the decomposition of the electrolyte and its reactions with both the anode and cathode produced combustible gases, further driving the battery into thermal runaway. This study aimed to investigate the impact of combustible vapors and gases on battery thermal runaway and designed a three-stage (EV+ accelerating rate calorimeter, ARC) testing procedure. In the first stage, we conducted a complete thermal runaway reaction test on an NCA 18650 battery with 100 % state of charge (SOC). The results exhibited that the safety valve opened at approximately 120 to 125 °C, and the temperature range before thermal runaway occurred was between 180 and 200 °C. These findings confirmed the characteristic temperatures before the valve opened and before thermal runaway. The second phase focused on the venting point and the temperature before thermal runaway. In order to gain a more precise understanding of the impact of combustible vapors and gas emissions on the overall thermal runaway process, we planned to implement external suction after the venting point. This would remove the combustible gases and maintain a stable environmental temperature, allowing us to verify whether removing the combustible gases could effectively delay the characteristic temperature points during the battery's thermal runaway process. The third stage involved adiabatic testing at various characteristic temperatures, with gas sampling taken when these temperatures were reached. The samples were analyzed using gas chromatography-mass spectrometry, to identify the types of combustible gases released at each characteristic point. Furthermore, we used the ideal gas equation to calculate the pressure collected at each stage and estimate the gas volume at the characteristic points, thereby revealing the state changes in the battery from valve opening to thermal runaway in terms of combustible vapor and gas generation. The ultimate goal of this study was to clarify the influence of combustible vapors and gases produced by the decomposition of the liquid electrolyte during thermal runaway on the thermal runaway process of the battery. It aimed to refine the understanding of the battery's thermal runaway mechanism further and render critical data for early warning and response strategies as an inherently safety measure.

Acknowledgments

Thanks to all colleagues of the Process Disaster Prevention and Laboratory (PS&DPL) for their assistance.

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Measuring nonequilibrium heat capacities

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Keywords: nonequilibrium calorimetry, negative heat capacity, ferroelectric material, AC calorimetry

Nonequilibrium calorimetry is a new and fascinating area where not only material but also functional properties can be explored using thermal response. We present the main procedures of nonequilibrium calorimetry, and how theory supports the experimental procedures and findings, representing an important step forward in nonequilibrium physics.

For the theoretical framework we refer to [1], where they consider stationary driven systems in contact with a thermal equilibrium bath. In these systems, when stationary, constant (Joule) heat is dissipated from the steady state to the thermal bath as long as all parameters remain unchanged. As a natural extension of the equilibrium situation, the nonequilibrium heat capacity measures the extra dissipated heat when the temperature of the thermal bath changes. To improve experimental accessibility, we demonstrate how heat capacity can also be obtained by measuring the response of the instantaneous heat flux to small periodic temperature variations. Specifically, we measure the heat capacity of the ferroelectric material TGS, while work (in terms of an oscillating electric field) is performed on the sample to create the nonequilibrium condition. The temperature of the bath oscillates at a small frequency, [2] which allows the thermal response. New features of nonequilibrium heat capacities include detection of dynamical phase transitions and negative effective temperatures.

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Hydration of biomolecules in the solid state: insights from isothermal and temperature scanning calorimetry

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Keywords: water sorption, hydration, differential scanning calorimetry, glass transition, sorption calorimetry

The primary industrial interest in water-biomolecule interactions in the solid state lies in their role in pharmaceutical formulations, particularly for biologics [1]. This topic also holds fundamental importance, as it allows for the investigations of concepts related to thermal behaviour of amorphous substances. In particular, carbohydrates used as excipients in pharmaceutical formulations serve as convenient objects for studying glass transition and water sorption behaviours.

Glass transition is a fundamental property of amorphous systems, which, when properly analysed, provides valuable insights into their physical characteristics. The simplest approach for describing the glass transition is the so-called "minimal model" [2], which based on two parameters offers a basic description of thermal properties in the glass transition region. Although too simplified for comprehensive understanding of the phenomenon, it is adequate for the description of glass transition in samples with certain thermal histories [3]. Thermal history is generally a crucial factor to control for correct interpretation of calorimetry and water sorption data on biomolecules in the solid state [3,4].

In glassy carbohydrates, water activity deviates from the expected equilibrium values, often leading to sorption-desorption hysteresis. The partial molar enthalpy of mixing of water (often referred to as hydration enthalpy) is negative in the glassy state and shows relatively complex profiles when studied by water sorption calorimetry [5,6]. This behaviour was recently explained based on the glass transition properties of the components [7]. To further develop this approach, we derived an expression for water activity in glassy materials, where the deviation from the equilibrium activity values is related to heat capacity changes of the components of the system [8].

Acknowledgments
VINNOVA, KK foundation and Sandberg Development are acknowledged for financial support.

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Study of phase transitions in supramolecular materials for third-order nonlinear optics

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Keywords: phase transitions, DSC, the influence of the heating rate and duration of the heating process, DDMEBT

The study of phase transitions in supramolecular materials, essential in third-order nonlinear optics, contributes to optimizing their performance in practical applications such as photovoltaic panels, optoelectronic devices, and advanced sensors [1, 2]. Polymorphism and solid-solid transitions, influenced by temperature and pressure, modify the crystalline structure, affecting the nonlinear response of materials. Additionally, sublimation deposition can cause successive phase changes (solid-gas-solid), influencing the material's stratification and optical characteristics [3]. Thus, understanding these transformations is crucial for controlling and improving the performance of supramolecular materials in advanced applications. In this study, we analyzed the influence of heating rate, preheating time, and temperature on the thermal behaviour of DDMEBT (2-[4-(dimethylamino)phenyl]-3-([4(dimethylamino)phenyl]ethynyl)buta-1,3-diene-1,1,4,4-tetracarbonitrile), a material with potential applications in optoelectronics. Using a differential scanning calorimeter DSC1 from Mettler Toledo, DSC curves were recorded with different heating rates of 1, 3.5, 5, 10, 15, and 20°C/min in the temperature range of 25–250 ºC or 270 ºC (Figure 1a). It was observed that the thermal behaviour changed with increasing heating rate. Variations in thermal characteristics after holding samples at different constant temperatures (60 and 80ºC) were also highlighted (Figure 1b). The results obtained reveal that heat treatment can convert the material to a more stable phase, with a lower melting enthalpy.

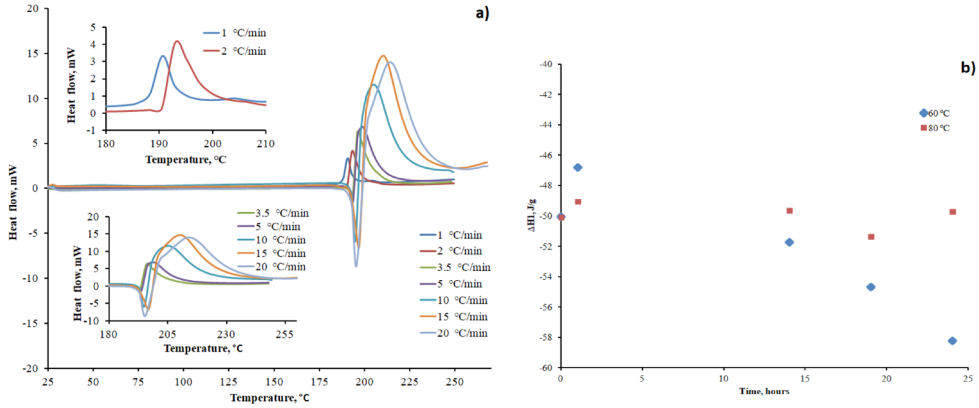

Figure 1. a) DSC curves at different heating rates; b) influence of time and temperature at which DDMEBT was preheated on the melting process

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Investigation of the thermal stability and degradation kinetics of hybrid polymer biocomposites reinforced with plant-derived additives

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Keywords: sustainable materials, thermal stability, thermal degradation, eco-friendly polymers, renewable raw materials

Polylactic acid (PLA) 4043D, an aliphatic polyester derived from renewable resources, has emerged as a strategically important biodegradable polymer within the circular economy, representing a sustainable and environmentally favorable alternative to traditional petroleum-based plastics. Its extensive utilization in diverse applications, including packaging, biomedical fields, and advanced functional composites, is primarily driven by its desirable mechanical properties, biodegradability, and ecological compatibility. Despite these advantages, PLA recycling is significantly hindered by intrinsic limitations related to thermal, hydrolytic, and oxidative degradation, constraining both reprocessing potential and long-term sustainability. PLA degradation encompasses intricate, multifaceted mechanisms such as thermal depolymerization, hydrolytic cleavage of ester bonds, and oxidative polymer chain scission. Collectively, these degradation pathways progressively decrease molecular weight, compromise mechanical performance, and diminish structural integrity during successive recycling cycles. Consequently, conventional mechanical recycling proves increasingly impractical due to the progressive deterioration of material properties, necessitating the exploration of advanced and innovative recycling approaches. Chemical recycling methods, particularly repolymerization, enable precise recovery of high-purity lactic acid or lactide monomers essential for synthesizing virgin-grade PLA. However, effective implementation of these processes demands meticulous control of reaction parameters and highly specialized catalytic systems. Recent scientific advancements in hybrid catalytic technologies significantly enhance selective depolymerization and monomer recovery efficiency, providing promising pathways for improving PLA recyclability. Additionally, reinforced recycling approaches employing bio-nanocomposites—such as silica nanoparticles, nanocellulose, or layered silicate additives—markedly enhance PLA's thermal stability, oxidative resistance, and overall secondary processability. Analytical characterization methods, notably Thermogravimetric Analysis (TGA) and Oxidation Induction Time (OIT) measurements, are critically important for systematically assessing the efficacy and stability improvements conferred by these advanced recycling strategies. Furthermore, enzymatic degradation techniques utilizing selective ester hydrolytic enzymes or lactohydrolases offer controlled and efficient degradation pathways, converting PLA into valuable monomeric or oligomeric intermediates. Integrating biotechnological methods with advanced chemical recycling techniques substantially enhances PLA lifecycle management, ensuring sustainable reintegration into material supply chains. Therefore, addressing PLA recycling challenges necessitates a multidisciplinary, integrated

strategy encompassing mechanical, chemical, biological, and analytical methodologies. The continued development and refinement of such comprehensive recycling technologies significantly reinforce PLA's pivotal role in promoting sustainability and advancing the circular economy paradigm.

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T03: Cements, building materials

Influence of micro-silica and superplasticizers on the hydration and rheological behavior of calcium aluminate cement

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Keywords: calcium aluminate cement (CAC), micro-silica, superplasticizer, calorimetry, hydration, rheology

The study investigates the early hydration and rheological properties of calcium aluminate cement (CAC) modified with micro-silica (MS) and different superplasticizers. The influence of MS content (5%, 10%, and 15%) and superplasticizers (FS and NT) on hydration kinetics and dynamic viscosity were analyzed. Isothermal calorimetry results indicate that MS significantly accelerates hydration, reducing the time to peak heat release. However, increasing MS content from 5% to 15% leads to a decrease in cumulative heat release. The effect of superplasticizers varies depending on the MS concentration: FS enhances early hydration but loses effectiveness over time, while NT maintains workability for up to 60 minutes. Rheological tests reveal that higher MS content increases viscosity, likely due to reduced free water. The combined use of FS and NT results in intermediate viscosity and workability. These findings provide insights into optimizing CAC mixtures for improved performance in construction applications.

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Production of low carbon dioxide clinker by using industrial wastes

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Keywords: carbon dioxide, clinker, waste, physico-mechanical properties

Cement clinker production needs high energy (about 1450°C) that produces a high amount of CO_2 emission [1]. Herein, Al-Dross waste has been used for reducing the energy required. Low energy clinker was prepared by mechanical mixing of calculated amounts of sand clay, limestone, iron ore and aluminum dross powders in appropriate weight ratios for 1 h in a ball mill. The dry mix has been fired at temperatures of 1380°C, 1400°C, and 1420°C using a suggested mix composition. Several characterization techniques have been studied such as XRD, SEM, particle size, density and compressive strength. The results show a complete conversion of free lime to calcium silicates and achieve the optimal cementing and strength properties at 1400°C, as confirmed by XRD analysis and compressive strength. The prepared cement was mixed in w/c ratio of 20% to produce a paste that is molded in cubic mold of 2.54 x 2.54 x 2.54 cm dimensions. Samples were casted to be tested for physical and mechanical properties. The density and compressive strength after 7 days of hydration are 1.9 g/cm^3 and 77.13 MPa, respectively.

The preparation of OPC clinker at a reduced temperature of 1400°C using minor amounts of iron ore and aluminum dross highlights the role of fluxing agents like Fe_2O_3 and Al_2O_3 in lowering the eutectic temperature, facilitating the formation of essential clinker phases such as C3S and C2S. The results obtained are expected to be promising in reducing the CO_2 emission through the reduction of ordinary firing temperature from 1450°C to 1400°C.

Acknowledgments
The authors acknowledge the financial support of Academy of Scientific Research (ASRT), Egypt for the project entitled: “Development and optimization of CO2 reduction technologies in cement industries".

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Insights into the hydration reactions of low-carbon cements

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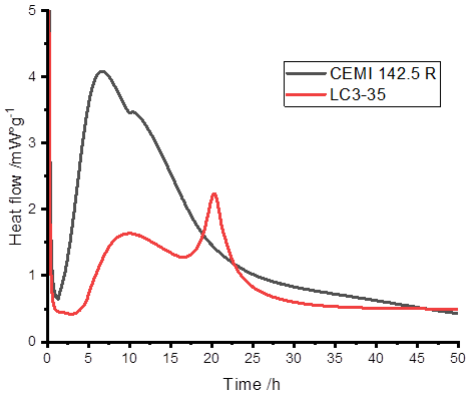
Keywords: hydration, products, kinetics, calorimetry, thermal analysis

Deepening the knowledge and understanding of the mechanisms and kinetics of hydration reactions of cement composites with a low to very low content of Portland clinker to develop low-carbon cements is currently and, in the future, the main focus of scientific research on inorganic composite binders. The construction sector, and in particular the manufacture of cement, contributes to global warming. To mitigate the detrimental effect of cement and concrete production on the environment, natural or artificial supplementary cementitious materials (SCMs) are combined with cement to produce low-carbon cements. The hydration reaction of cement is a complex process, even more so in a system containing SCMs. Further improvement of the required technical properties of cements is conditioned by sufficient knowledge of the basic chemical and physicochemical processes during the hardening of cement binders. In the present work, the hydration reactions of low-carbon cements based on binary, ternary, quaternary, and five-component mixtures comprising 50, 40, and 30 % of OPC and LC3(Limestone calcined clay cements are a family of blended cements that incorporate limestone and calcined kaolinitic clays, replacing up to 50% of clinker) alongside pure Portland cement were investigated using conduction calorimetry, thermogravimetry, and XRD methods. The main SCMs used were blast-furnace slag (BFS), finely ground limestone (GL), metakaolin (MK), silica fume (SF), and a special mixture (CYMENT). Considering the calorimetric curves of 48-100-hour hydration, it is evident that the overall hydration heat is reduced proportionally to the content of OPC in the mixtures. Due to the lack of $Ca(OH)_2$ resulting from the hydration of C_3S and C_2S, the results of alkali activation reactions are less intense. However, the effect of adding SCMs is evident in the second peak, which has a higher intensity than the first in low-carbon cements. While the hydration of OPC remains more progressive over time, new hydration products form in low-carbon cements, enhancing mechanical and physical properties and making mortars based on low-carbon cements more durable than those made with OPC.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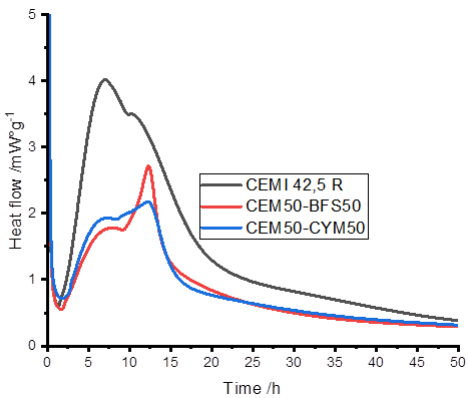
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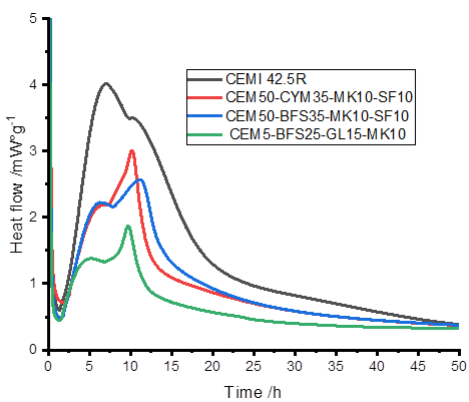
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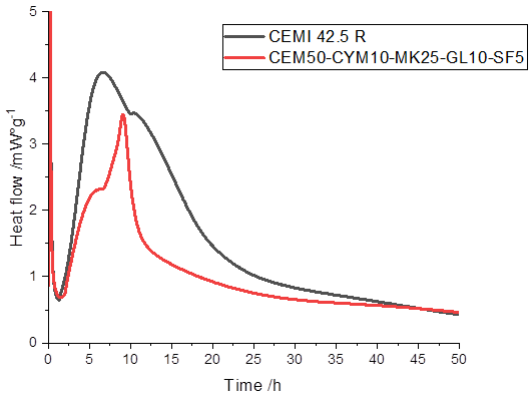
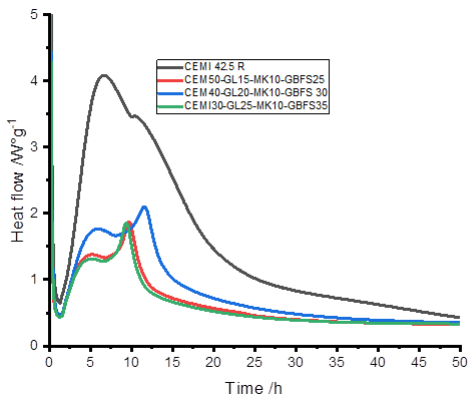
CEM5-BFS25-GL15-MK10
Heat flow /mW*g-1
Time /h

C



D



E

Fig. 1 Heat flow of different low-carbon cement compared to CEM I 42,5 R

Acknowledgments

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Characterization of carbonated wollastonite-based clinker by thermal analysis and isothermal calorimetry

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Keywords: carbonation curing, CCU technology, wollastonite-based clinker, supplementary cementitious materials

The cement industry is constantly aiming to reduce carbon dioxide emissions. The most commonly used techniques include the production of blended cements (with the addition of various supplementary cementitious materials, SCMs), the use of alternative fuels, and the production of low-emission binders. Currently, the greatest potential is seen in carbon capture and storage (CCS) technology, as well as, moving further, in carbon capture and utilization (CCU) technology [1].

Calcium silicates, such as wollastonite, rankinite, and ɣ-dicalcium silicate, do not bind in alkaline environments. However, they are readily subject to forced carbonation processes, making them useful as SCMs in cementitious systems [2]. A material based on non-binding calcium silicates - wollastonite and rankinite - has been described as wollastonite-based clinker or calcium silicate clinker.

Wollastonie-based clinker was burned in a semi-industrial rotary kiln with a capacity of approximately 50 kg/h at 1240°C using secondary raw materials. The obtained material was treated with mineral carbonation [3].

In the following studies, carbonated (CSc) and non-carbonated (CS) wollastonite-based clinker was used as a SCM to replace 30 % of clinker (by weight) in Portland cement. CEM I 52.5R was used as a reference sample. Samples with the most commonly used SMCs, i.e. granulated blast furnace slag and fly ash (clinker:SCM weight ratio of 70:30), were also made for comparison. The sample with carbonated wollastonite-based clinker (CSc) shows a lower compressive strength compared to the reference sample, but its value oscillates at the level of the strength of the sample with 30%wt. fly ash addition. Phase composition analysis (XRD) and thermogravimetric analysis (TGA) were also performed after different curing periods (hydration experiments) for samples with carbonated (CSc) and non-carbonated (CS) clinker. XRD analysis showed the presence of phases typical of the reacting cement. Samples with non-carbonated wollastonite-based clinker (CS) show a high content of wollastonite and rankinite even after 180d hydration, which is not observed for samples with carbonated clinker (CSc). TGA analysis showed a decrease in portlandite content during the hydration progression for the sample with carbonated clinker (CSc). This indicates the pozzolanic properties of the carbonated material. Isothermal calorimetry studies have shown that carbonated clinker (CSc) accelerate early hydration and cumulative heat of CS after 7 days is higher than for CSc.

Acknowledgments
This research has been supported by the Łukasiewicz Research Network, under Łukasiewicz Research Internship 2024.

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Tg and xrd characterisation of the phases develeped in heat cured pastes susceptible to delayed ettringite formation (DEF)

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Keywords: delayed ettringite formation (DEF), heat cured cement paste, TG, XRD

Delayed ettringite formation (DEF) is a deleterious reaction that can occur in heat cured or mass poured concrete [1]. Typically, DEF occurs when conditions promote decompositions of ettringite in the early stages of curing, but promote ettringite precipitation at a later age when the concrete is in its hardened state. As ettringite is an expansive phase, its precipitation has the potential to cause cracking and hence deterioration of the concrete and is a potential issue in heat cured precast concrete elements as well as in mass pours.

For DEF to occur, pessimum conditions are required which include elevated sulphate (≈ 4% SO_3) and alkali ion (Na^+, K^+, ≈ 1% Na_2O_e) content and elevated temperature (>70 °C) curing. The elevated alkali content and elevated temperature inhibit the formation and promote the decomposition of early ettringite in the setting period of the concrete when the concrete is in its plastic state and can accommodate the precipitation of an expansive phase. After curing and once the temperature has returned to ambient, the process of ettringite precipitation is initiated, however, at this point of the curing cycle, the concrete is in its hardened state and is less able to accommodate the precipitation of an expansive phase resulting in stress applied to the concrete leading to brittle failure and cracking.

Minimisation of the risk of DEF in precast concrete is achieved by specifying the temperature limits within the concrete during curing and by applying compositional limits in sulphate and alkali content (Na_2O_e) which, in Australia, are typically 70 to 80°C, 0.6% Na_2O_e and 3 to 3.5% SO_4^{2-}, but vary by jurisdiction. A unified approach to specification across the jurisdictions of Australia requires investigation of the role of these factors in the risk of DEF. These have been investigated and reported for expansion tests by our group in [2] which demonstrated that, if the sulphate and alkali content is maintained below 3% SO_3 and 1% Na_2O_e, elevated temperatures up to 90°C could be applied to the curing without risk of deleterious expansion.

In order to investigate the origins of these observations, a study into the phase development was carried out. The results of the phase development in cement pastes and 'grouts' containing fine ground aggregate as a function of sulphate (% SO_3) and alkali (Na^+, K^+, % Na_2O_e) content and curing temperature using TG and XRD for up to two years of aging at ambient temperature after subjecting the specimens to a range of curing programs are reported and discussed in the context of the primary factors responsible for DEF in the phase development.

Acknowledgments
This research was funded through an Australian Research Council Research Hub for Nanoscience Based Construction Materials Manufacturing (NANOCOMM) with the support of the Cement Concrete and Aggregates Australia (CCAA). The authors are grateful for the financial support of the Australian Research Council (IH150100006) in conducting this study. This research is supported by an Australian Government Research Training Program Scholarship.

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Influence of granulated blast furnace slag and silica fly ash on the hydration kinetics of multi-component cements

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Keywords: cement hydration, fly ash, blast furnace slag

This paper presents the results of microcalorimetric and conductometric studies on the hydration kinetics of multicomponent cements containing granulated blast furnace slag and silica fly ash. For this purpose, alite mixtures with a variable ratio of silica fly ash to granulated blast furnace slag were prepared. The studies were carried out using a differential microcalorimeter, with a water-binder ratio of 0.4. Analysis of microcalorimetric curves showed that increased fly ash content extends the induction period and delays the occurrence of heat release peaks. Reducing the alite share in the cement composition results in a decrease in the total heat of hydration, but this relationship is not linear. The decrease in the heat of hydration at 70% alite replacement is about 50%, which suggests an additional thermal effect resulting from the interaction of slag and ash with hydration products. The lowest value of the heat of hydration after 168 h was recorded for cement containing 40% of silica fly ash and 30% of granulated slag, while the highest for cement containing 30% V and 40% S, respectively. The test results confirm that a higher share of granulated blast furnace slag in relation to fly ash accelerates the occurrence of the maximum in the post-induction period, which may be of significant importance in the design of cements with controlled reactivity.

Research on the compressive strength of micp-modified aggregate concrete mixed/cured with salt water

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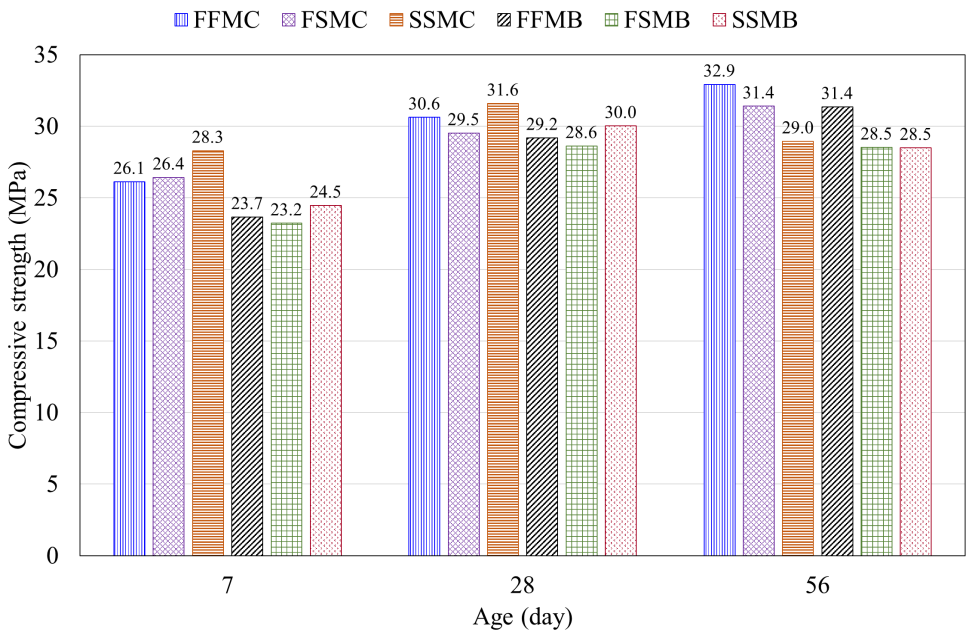
Keywords: MICP, self-healing, concrete, compressive strength, salt water, recycled aggregate

In order to understand the development of compressive strength of MICP-modified aggregate concrete mixed/cured with salt water, this study referred the research [1-3] to use waste red brick aggregates (RBA) and crushed concrete aggregates (CCA) via the technology of microbial-induced calcium carbonate precipitation (MICP) to improve their pore structure. Then, these aggregates were used to replace natural coarse aggregates and produce concrete for compressive strength testing. Figure 1 shows the result of the compressive strength test. It can be found that the 7-day and 28-day compressive strengths of the SSMC concrete are higher than those of the other concrete. However, SSMC concrete has the lowest compressive strength compared to other CCA concrete at a later age (56-day), even lower than FFRB concrete. This indicates salt water curing/mixing can enhance the compressive strength of modified aggregate concrete before the age of 28 days. However, it is not conducive to the strength development of concrete at a later age. This phenomenon is also found in the test result of the RBA concrete series. Because the large pore structure of RBA is more significant than that of CCA, the effect of MICP-modified RBA is insignificant. Hence, the increment/reduction of compressive strength of SSMB concrete at an early/later age compared to that of FFMC is smaller than that of SSMC.



Note

FFMC: fresh water mixing/curing modified crush aggregate concrete;
FSMC: fresh water mixing and salt water curing modified crush aggregate concrete;
SSMC: salt water mixing/curing modified crush aggregate concrete;
FFMB: fresh water mixing/curing modified brick aggregate concrete;
FSMB: fresh water mixing and salt water curing modified brick aggregate concrete;
SSMB: salt water mixing/curing modified brick aggregate concrete.

Figure 1 Development of compressive strength of modified aggregate concrete.

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Thermal activation and pozzolanic reactivity of estonian clays for cementitious applications

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Keywords: illite-rich clay, thermal activation, pozzolanic activity

Supplementary cementitious materials (SCMs) are pivotal in mitigating CO_2 emissions from cement production [1]. This study evaluates the pozzolanic reactivity of locally sourced clays from Estonia as emerging sustainable SCM alternatives [2]. Three non-kaolinitic clays (from Kunda, Arumetsa and Aseri deposits) are characterized comprehensively, encompassing physical properties (particle size distribution, specific surface area, Blaine fineness, and density) and chemical/mineralogical analyses (X-ray fluorescence and X-ray diffraction), as well as thermal transformation assessments. Thermal activation is conducted in a rotary tube furnace at 750, 825, and 900 °C with a 60-minute residence time—emulating small-scale rotary kiln conditions. The pozzolanic activity of the thermally treated clays is initially evaluated through alkali leaching tests using NaOH suspensions, with the electrical conductivity and dissolution of silicon (Si) quantified. Subsequent mechanical performance was assessed by 28-day compressive strength tests on lime-based mortars (EN 196-1), and thermogravimetric analysis is employed to determine the bound water content in hydration products. The most promising calcined clays were further tested as partial replacements for cement and sand, with isothermal calorimetry utilized to elucidate hydration kinetics and strength development. The concentrations of dissolved Si are found to be dependent on the clay mineralogy (contents of illite, smectite, and kaolinite), and correlate with the observed pozzolanic reactivity of the calcined clays. Both elemental dissolution and pozzolanic reactivity increase with rising calcination temperatures and mechanochemical activation for Kunda and Aseri, though only up to an optimal threshold. While early hydration stages exhibit minimal reactivity, a significant degree of reaction occurs with prolonged hydration of Arumetsa sample. These findings highlight the potential of locally available illite-rich clays—with moderate pozzolanic reactivity—as sustainable and accessible supplementary cementitious materials.

Acknowledgments
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T04: Ceramics, glasses

Influence of the crystallization process on the properties of bulk metallic glasses $MG_{66}ZN_{30}CA_4$

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Keywords: crystallization, bulk metallic glasses, magnesium alloys

Metallic glasses based on magnesium with a chemical composition of Mg-Zn-Ca can be considered as a potential biomaterial due to the single-phase structure. Gu and others studied the mechanical properties and corrosion resistance of Mg–Zn–Ca alloys. The tests conducted suggested their high compressive strength, above 500 MPa, which is three times higher than that of pure magnesium, while the corrosion research indicated high corrosion resistance. It can therefore be assumed that the amorphous structure of metallic glasses may provide a material with higher corrosion resistance and better mechanical properties, such as high strength and hardness, than crystalline materials. However, the widespread use of amorphous alloys is limited due to their low plasticity. Creating a composite structure with glassy and crystalline phases can increase plasticity. However, achieving an amorphous structure with a larger cross-section can be very difficult. An important parameter in obtaining metallic glasses is the glass-forming ability (GFA). It is worth mentioning that materials with a mixed structure (amorphous-crystalline) can still exhibit good plastic properties and corrosion resistance. Therefore, it is crucial to understand the crystallization kinetics of magnesium-based metallic glasses. Consequently, it is necessary to investigate the effect of annealing temperature on the structure and properties of magnesium-based amorphous alloys and their potential implant applications.

Ablation resistance of titanium diborate based composites obtained viareactive sintering

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Keywords: titanium diboride, composites, ablation, spark plasma sintering, intermetallics

"The study's focus on TiB-TiC-SiC composites produced through reactive sintering using the SPS technique represents a significant advancement in the development of high-temperature materials. By combining intermetallic compounds from Ti-Si and Ti-Al systems with B-C and C, the researchers have created composites with exceptional properties. The sintering temperature range of 1000 to 1700°C allows for precise control over the material's microstructure and properties, enabling the optimization of processing conditions for specific applications. The comprehensive characterization methods employed, including density measurements, XRD analysis, and X-ray absorption spectroscopy, provide a thorough understanding of the composites' structure and composition, which is essential for predicting and improving their performance.\n\nThe ablation resistance test, conducted using an oxyacetylene flame at 1800°C for 60 seconds, offers a practical assessment of the material's performance under extreme conditions, simulating the harsh environments encountered in aerospace and industrial applications. The use of confocal microscopy and SEM/EDS for post-ablation analysis enables a detailed examination of the ablation zone and chemical changes occurring during high-temperature exposure, providing valuable insights into the material's behavior and degradation mechanisms.

The strong ablation resistance demonstrated by these composites, particularly when compared to commercially available materials, underscores their potential for use in demanding applications where high-temperature resistance is critical. This research not only contributes to the development of next-generation materials capable of withstanding extreme environments but also opens up new possibilities for improving the efficiency and durability of components in various technological fields, such as aerospace, energy production, and advanced manufacturing."

Acknowledgments
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Batio$_3$ ceramics: advances in synthesis methods and SPS sintering strategies

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Keywords: BaTiO3 ceramics, solid state reaction, modified Pechini synthesis, spark plasma sintering

Barium titanate ($BaTiO_3$) ceramics are widely studied due to their excellent dielectric properties, making them essential for applications in capacitors, sensors, and energy storage devices. The growing demand for high-performance ferroelectric materials necessitates the optimization of synthesis and sintering techniques to achieve desirable microstructures and functional properties.

In this study, $BaTiO_3$ ceramics were synthesized using two distinct methods: the Pechini method, which enables fine particle control through a polymeric precursor route, and the conventional solid-state reaction, which is widely used for large-scale production but often results in coarser particles. To evaluate the effects of different sintering techniques, both conventionally sintered and Spark Plasma Sintered (SPS) $BaTiO_3$ samples were prepared. Conventional free sintering relies on diffusion-driven densification at high temperatures over extended times, which can lead to grain growth and porosity. In contrast, SPS employs pulsed direct current and applied pressure to accelerate densification, allowing for lower sintering temperatures and shorter sintering times while limiting grain growth. By varying key parameters such as sintering temperature, applied pressure, and dwell time, the study aims to determine how these factors influence the final microstructure and functional properties of $BaTiO_3$ ceramics.

The obtained materials were characterized using X-ray diffraction (XRD) to analyze phase composition, scanning electron microscopy (SEM) to assess microstructure and grain size distribution, differential scanning calorimetry (DSC) to study thermal behavior, and dielectric permittivity measurements to evaluate electrical properties. The results provide a comparative analysis of the impact of synthesis and sintering techniques on $BaTiO_3$ ceramics, highlighting key differences in phase stability, densification behavior, and dielectric response. Special attention will be given to the trade-offs between high-density ceramics and controlled grain growth, which are critical for tailoring materials to specific applications.

By systematically examining the relationships between synthesis, sintering conditions, and material properties, this study contributes to a deeper understanding of $BaTiO_3$ processing and offers insights into optimizing ceramic fabrication for advanced technological applications.

Acknowledgments
This work was funded by the Priority Research Area Excellent Small Working Groups under the program “Excellence Initiative – Research University” at University of the National Education Commission,.

Vanadium-doped mesoporous bioactive glasses as potential targeted therapy for osteosarcoma

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Keywords: mesoporous bioactive glasses (MBGs), vanadium (V_2O_5), osteosarcoma, antitumor activity

Cancer is a life-threatening disease affecting humans, with its prevalence steadily rising worldwide. Developing innovative approaches for cancer therapy is a continuous process, and mesoporous bioactive glasses (MBGs) showed excellent potential for this purpose. In this study, MBGs within the (70-x)SiO_2–26CaO–4P_2O_5-xV2O5 (x=0, 0.5, 1 mole %) system were synthesized by evaporation-induced self-assembly (EISA) method. V_2O_5 was suggested because it promotes osteogenesis and enhances cellular responses. X-ray diffraction (XRD), Fourier-transform infrared (FTIR), scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), thermogravimetric analysis (TGA), differential scanning calorimetry (DSC) were used to evaluate the structure, morphology, composition, and thermal properties of the investigated samples. The pore size of 5 nm confirms the mesoporosity of the glass, while the valence state of vanadium ions ($V4^+/V^{5+}$) was determined using UV-Vis spectroscopy. The antitumor evaluation of the investigated MBGs on the Saos-2 osteosarcoma cell line, assessed using the MTT assay, demonstrated an antiproliferative effect. A significant inhibition rate of over 50% at 125 μg/mL concentration was observed for the glass with higher vanadium content. The results show that investigated MBGs have potential for cancer treatment in bone regeneration.

Acknowledgments
The data presented in this study will be utilized as part of a doctoral thesis.

Effect of ZrO_2 addition on thermal behavior and structure of Y_2O_3-Al_2O_3-ZrO_2 ternary glasses with eutectic composition

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Keywords: Y_2O_3-Al_2O_3 eutectic composition, Pechini sol-gel, flame spraying synthesis, thermal properties

Al_2O_3-YAG-ZrO_2 eutectic composites demonstrate high strength, thermal stability, creep resistance, and corrosion resistance at elevated temperatures (up to 1600 °C), making them suitable for high-temperature applications. However, their preparation is both financially and technologically demanding. The controlled crystallisation of yttria-aluminate glasses with ZrO_2 addition provides a potential solution. Nonetheless, the fabrication of these glasses necessitates specialised melting equipment, primarily due to their high melting temperatures and significant tendency to crystallise. Producing glass microspheres via flame synthesis and their subsequent sintering seems to be a promising approach.

The aim of this work was to prepare and characterise glasses using flame spraying synthesis in the Y_2O_3-Al_2O_3 system with varying amounts of ZrO_2 added. The precursor powders used for flame synthesis were prepared by the Pechini sol-gel method to ensure high homogeneity. The eutectic composition of the Y_2O_3-Al_2O_3 system was selected as the basis, i.e. 76.8 mol% Al_2O_3 and 23.2 mol% Y_2O_3. The molar ratio of Al_2O_3/Y_2O_3 was maintained constant while the ZrO_2 content increased from 5 to 20 mol. % (5,10, 15 and 20 mol. %). The phase composition, thermal behaviour and structure of the prepared glasses were examined using X-ray diffraction (XRD), scanning electron microscopy (SEM), differential scanning calorimetry (DSC), high temperature X-ray diffraction (HT-XRD) and ^{27}Al MAS NMR.

The prepared glasses with lower ZrO_2 content (5 and 10 mol.%) were X-ray amorphous. In contrast, the glasses with higher ZrO_2 content (15 and 20 mol.%) were partially crystalline, and traces of crystalline ZrO_2 were observed in the XRD patterns. This result aligned well with the SEM investigation. Samples with lower ZrO_2 additions primarily contained smooth, fully remelted particles without signs of crystallisation. In the case of samples with higher ZrO_2 content, a small proportion of partially or fully crystalline microspheres was noted. DSC records of all prepared glass microspheres contained two exothermic peaks. A similar behaviour was observed for the undoped Y_2O_3-Al_2O_3 eutectic composition [2]. The first peak was noted around 935 °C for all compositions. The second exothermic peak ranged from 1000 °C for the sample with the lowest ZrO_2 content to 1190 °C with the highest sample. The temperature difference between the two exothermic events increases with higher ZrO_2 content. HT XRD confirmed crystallisation in the observed interval (750-1200 °C). For the

sample with the lowest ZrO_2 content, the YAG phase crystallised at 920 °C, similar to what was observed in yttrium-aluminate glasses in our previous work [2]. In samples with higher additions (10 mol.% and more), ZrO_2 crystallisation was observed first (monoclinic or tetragonal), followed by YAG crystallisation. The preferential crystallisation of ZrO_2 in these samples may be attributed to trace amounts of these phases in the samples after flame synthesis, which may act as nucleation centres. Al2O3 crystallisation (θ-Al_2O_3 or α-Al_2O_3 form), which was noted as a competitive process to YAG crystallisation in Y_2O_3-Al_2O_3 glasses [2], was not observed. Finally, ^{27}Al MAS NMR spectra of the prepared glasses were measured, and the role of ZrO_2 in the structure of the Y_2O_3-Al_2O_3 glasses was discussed.

Acknowledgments
The financial support of this work by the projects VEGA 2/0077/24 and VEGA 2/0104/25 is gratefully acknowledged.

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Impact of SrO addition on the structure and thermal properties of the floor tile glazes with CaO/MgO changing molar ratio

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Keywords: glass-ceramic materials, floor tiles, hot stage microscopy, dilatometry, differential scanning calorimetry

The experiment aimed to check how the addition of strontium oxide affects the thermal properties of glazes intended for floor tiles. For this purpose, two oxide systems SiO2-Al2O3-Na2O-K2O-CaO/MgO were designed, one containing calcium oxide, and the other magnesium oxide. To each of these systems, strontium oxide (as strontium carbonate) was added in amounts of 2.5, 5 and 7.5 of this oxide. The glazes obtained were prepared by wet grinding natural raw materials (raw type glazes) and then examined using a high-temperature microscope (HSM). The results obtained were used to determine the firing temperature. The fired glazes were subjected to microstructure observations (SEM-EDS) and phase composition determination (XRD). The raw powders were used for thermal measurements using a mechanical dilatometer (DI) and differential scanning calorimetry (DSC) and for measurements of structural changes using mid-infrared spectroscopy (MIR). The effects determined using DSC were identified by heating the raw powder to the effect temperature, then rapidly cooling it and determining the phase composition using X-ray diffraction. The results were compared, and as a result, information was obtained that indicates how the addition of strontium oxide affects the structure and the thermal effects in the two analysed systems.

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$Al_2O_3/Y_3Al_5O_{12}/ZrO_2$ glass-ceramics the influence of composition on thermal properties and sinter ability

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Materials with eutectic microstructure in binary (Al_2O_3-Y_2O_3) or ternary (Al_2O_3-Y_2O_3-ZrO_2) systems have been intensively investigated due to their excellent mechanical properties, which they retain even at high temperatures (up to 1600°C). However, their preparation by controlled crystallization from melt is financially and technically demanding and limited to small sample volumes. A combination of flame synthesis and commercially available sintering methods such as hot-pressing, hot-isostatic pressing, rapid hot pressing and spark plasma sintering appears to be an economically advantageous solution of their production, at much reduced temperatures in comparison to melt crystallization. Glass ceramics materials in the Al_2O_3-Y_2O_3 system have been successfully prepared by the combination of the pressure assisted sintering methods, with very fine- grained defect-free microstructure and relatively high values of H_v=17.6±0.2 GPa and K_{IC}=4.2±0.3 MPa.$m^{1/2}$. In this work, four glass compositions in the system Y_2O_3-Al_2O_3-ZrO_2 were prepared in the form of glass microspheres using the flame spraying method. The composition of the prepared glasses was derived from the eutectic composition of the Al_2O_3-Y_2O_3 system (76.8 mol.% of Al_2O_3 and 23.2 mol.% of Y_2O_3), where 5 and 10 mol.% of Al_2O_3 were replaced with ZrO_2 in the SZr1 and SZr2, and 5 and 10 mol.% of Y_2O_3 were replaced with ZrO_2 in the SZr3 and SZr4 compositions respectively.

XRD analysis confirmed the XRD amorphous nature of the systems SZr1-SZr3 and partially crystalline nature of the SZr4. Three exothermic effects with maxima in the interval 937 – 1142 °C were observed in DSC curves of SZr1-SZr3. Only one exothermic effect with the maximum at 939 °C was observed in the DSC curve of SZr4. To obtain the most comprehensive information about phase development during thermal annealing of systems, high temperature XRD analyses in the temperature interval 750-1450°C were performed. A comparison of XRD patterns showed mainly the crystallization of YAG ($Y_3Al_5O_{12}$) and ZrO_2 phases (monoclinic and tetragonal) in the temperature interval 980-1200°C, with the onset of ZrO_2 phases crystallisation at 980°C. The YAG phase began to form at temperatures around 1080°C. Also, slow crystallization of the intermediate Al_2O_3 phase (θ-Al_2O_3 ; T~1100°C) after careful examination of XRD patterns. Crystallization of α-Al_2O_3 was detected up to 1300°C. The preliminary hot-press experiments were performed at a temperature of 1500°C, pressure of 30 MPa and with an isothermal dwell of 10 min. Very fine eutectic microstructure, created by YAG and ZrO_2 grains embedded into α-Al_2O_3 matrix, and a high level of homogeneity was

observed by SEM and SEM EDX. Vickers hardness (H_V = 17.8±0.4 GPa) and the indentation fracture toughness K_{IC} = 4.6±0.3 MPa.$m^{1/2}$ were determined by Vickers indentation (load of 10 N; dwell time 10 s) in SZr3.

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T06: Energetic materials

Thermal and radiation ageing evaluation of nuclear cables using DSC

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Keywords: nuclear cable ageing, maintenance diagnostic testing, Indenter Modulus (IM), Differential Scanning Calorimetry (DSC)

During operation of nuclear power plant (NPP), there are many electrical, thermal, radiation, humidity and mechanical stresses, which can influence degradation of cable insulation. Thermal and radiation degradation mechanism are common and specific combination for NPP that might lead to ageing effects and early degradation of polymers used in electrical cables. Electrical cables are important component in NPP and it is mandatory to monitor their functionality. Accordingly, it is necessary to select effective diagnostic methods to determine functionality, reliability, and possible degradation due to various influencing factors and aging of cable insulation. To avoid unplanned failures with loss of critical and important safety equipment, the insulation must be properly tested. Different electrical and non-electrical diagnostic methods are used to ensure proper assessment of cable insulation. Initial Cable Aging Management Program (CAMP) was implemented in Krško NPP in 2010 as one of requirements for plant life extension above 40 years of operation. Assessment of the condition of cable insulation is supposed to be carried out periodically, during the maintenance activities. The diagnostic testing and measurements on cables are required respecting regulations, standards and a good practice of asset maintenance management is discussed. This paper reports on experience with application of different mechanical and chemical diagnostic methods for monitoring of the condition of the cable insulation in the Krško NPP. The article presents results of cable insulation testing mechanical and chemical properties such as Indenter Modulus (IM) and Differential Scanning Calorimetry (DSC). DSC was recognised as appropriate thermoanalytical laboratory technique due to very small sample needed for analysis. Experiments were performed on different nuclear "1E" cables with most frequently used polymer materials such as ethylene propylene rubber (EPR) and crosslinked polyethylene (XLPE) all with chlorosulphonated (CSPE) jacket. Cable samples, old between 10 to 40 years, were selected from warehouse and additionally thermal-aged in nine different steps at a high temperature of 120 °C. The results were compared with the results of simultaneous radiation ageing in combination with a moderate temperature of 50 °C, where the samples were irradiated with total radiation doses of 500 kGy, 1000 kGy, 1500 kGy and 2000 kGy. Deviations due to radiation ageing effects were searched and results reported. Some results showed an evident change of properties in nuclear cables polymers and could be used to determine acceptance criteria and evaluation of functionality prediction models.

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Determination of crucial thero-mechanical parameters of solid rocket propellants after long-time storage in terms of operational safety

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Keywords: solid rocket propellants, thermo-mechanical analysis, glass transition

The paper presents experimental research on the thermomechanical properties of solid homogeneous rocket propellant used in anti-tank guided missiles, after long-term storage, with the use of modern analytical tools. A periodic control testing system for munitions and explosives is essential for maintaining the state's self-defense capabilities. The investigated parameters of the propellant include the thermal decomposition temperature, glass transition, softening temperatures, and the coefficient of thermal linear expansion. These characteristics are essential for the safe operation of rocket motors. The temperature changes to which a rocket motor may be subjected during storage and operation can cause stresses to appear in the rocket propellant grain. This may lead to cracking of the material and, consequently, an uncontrolled increase in the combustion surface, which can result in a sudden increase in pressure in the combustion chamber and, in the worst case, an explosion of the missile during launch. Therefore, conducting comprehensive studies of the thermomechanical properties of stored propellants is necessary, using reliable tools that provide repeatable results. The thermal decomposition of the propellant was determined using the TA Instruments Discovery DSC 250 and Discovery TGA 5500, with a heating rate of 10 K/min for both methods. The results of calorimetric and gravimetric analysis provide the upper temperature limit for the mechanical analysis, in which the samples of the propellant are much larger. The mechanical characteristics of the tested propellant were determined using the Netzsch Dynamic Mechanical Analyzer DMA 303 Eplexor device, in the temperature range from -120°C to 100°C, with a heating rate of 2 K/min. The glass transition temperature was determined according to the STANAG 4540 agreement. Thermal linear expansion was studied using the Netzsch Thermo-mechanical Analyzer TMA 402 F3 Hyperion in the temperature range from -100°C to 80°C, with a heating rate of 3 K/min. Both mechanical analysis techniques show compliance in the results of glass transition and softening temperatures.

Microcrystalline graphite extraction process from low grade graphite ores using surfactant

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Keywords: microcrystalline graphite, graphite extraction, graphite beneficiation, energy storage material

Graphite is a critical material with diverse industrial applications, including steelmaking, refractories, metallurgical processes, and, most importantly, lithium-ion (Li-ion) battery electrodes. With the increasing demand for Li-ion batteries in electric vehicles (EVs), the global demand for graphite is surging, influencing market dynamics and geopolitics. As the need for faster charging batteries grows, microcrystalline graphite has emerged as a superior material due to its smaller particle size, which enhances ion transport and electrochemical performance[1]. However, graphite ore is naturally associated with various impurities, necessitating beneficiation before industrial use. The widely used froth flotation method does not extract fine-sized graphitic particles, leaving microcrystalline graphite ores underutilized despite their abundance. This study presents a surfactant-assisted separation method for selectively extracting microcrystalline graphite flakes from low-grade ore. The ore was initially characterized using X-ray Diffraction (XRD) to identify mineral phases, Energy Dispersive X-ray Spectroscopy (EDX) for elemental composition, Raman Spectroscopy for carbon characterization, Thermogravimetric Analysis (TGA) for thermal stability, and Field Emission Scanning Electron Microscopy (FESEM) to examine morphology and particle size. The ore powder was sonicated in a Sodium Dodecyl Sulfate surfactant aq. solution, followed by centrifugation, separated a stable supernatant rich in graphitic particles and unstable settled particles, primarily composed of inorganic impurities. The supernatant was vacuum-filtered and dried, and both fractions were subsequently characterized. EDX analysis revealed a significant enrichment of carbon content, increasing from 13.2 at. % in the raw ore to 51.4 at. % in the supernatant fraction. FESEM confirmed that the extracted graphitic flakes were smaller than 2 microns, aligning with the desired microcrystalline particle size. Raman spectroscopy further validated the successful separation, as the quartz peaks observed in the raw ore were absent in the supernatant fraction. This novel surfactant-assisted approach demonstrates an efficient, scalable, and eco-friendly method for beneficiating microcrystalline graphite, unlocking its potential for energy storage applications, including next-generation fast-charging Li-ion batteries.

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Thermal stability and decomposition mechanism of nitrocellulose

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Keywords: energetic materials, spontaneous decomposition, thermal safety, heat flow calorimetry

Nitrocellulose (NC), a nitric acid ester compound containing an ONO_2 functional group, is widely utilized as a raw material in explosives, lacquers, and celluloid products. Although NC has a wide range of industrial applications, it is highly unstable and prone to spontaneous decomposition even at low temperatures. The accumulation of decomposition heat can lead to spontaneous ignition, posing a risk of severe accidental explosions[1]. While the spontaneous decomposition of NC has been investigated for many years, recent incidents seem to have renewed interest in understanding its reaction mechanisms and improving safety measures based on scientific evidence. Previous studies have shown that reactive species such as O_2 and H_2O in the surrounding environment, as well as NO_2 and HNO_3 generated from NC itself, accelerate its exothermic decomposition[2]. However, the detailed reaction mechanisms remain to be fully elucidated. This study aims to clarify the role of these reactive species in the spontaneous decomposition of NC and to contribute to a more comprehensive understanding of its decomposition pathways. To achieve this, the authors performed heat flow calorimetry on NC at heating rates of 0.05 K/min or lower in air and N_2 atmospheres with the addition of NO_2, H_2O, and HNO_3. This experimental approach enabled the evaluation of the effects of different reactive species on the decomposition behavior of NC. The experimental results revealed distinct effects of each additive on NC decomposition. Specifically, NO_2 lowered the decomposition temperature of NC only in air. In an N_2 atmosphere, the decomposition behavior remained unchanged regardless of the presence or absence of an excessive amount of NO_2 (5,000 ppm), suggesting that the effect of NO_2 on NC decomposition depends on the presence of O_2. In contrast, both H_2O and HNO_3 lowered the decomposition temperature in both air and N_2 atmospheres, with HNO_3 exhibiting a more pronounced impact than H_2O. These findings suggest that while NO_2 alone cannot sustain radical chain reactions without O_2, the formation of HNO_3 during NC decomposition and its conversion from NO_2 in the presence of H_2O may be crucial for maintaining these reactions. Furthermore, our quantum chemistry studies, based on first-principles calculations, propose a decomposition mechanism for an NC model compound (NC_m) that includes the generation pathways of NO_2 and HNO_3, as well as their interactions with NC_m in the presence of O_2. The experimentally observed thermal behaviors in this study align with the proposed mechanism, supporting its validity.

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Sb_2S_3 thin films by ultrasonic spray in air: formation and application in solar cells

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Keywords: antimony sulfide, ultrasonic spray, metalorganic precursors, thermal analysis, solar cell

Sb_2S_3 with bandgap of 1,7 eV, absorption coefficient $1 \cdot 10^5$ cm^{-1} at 450 nm and good stability makes it prime candidate for application as top cell absorber layer in tandem solar cells, and as an absorber in semitransparent cells for building integrated applications or in cells used for powering of IoT devices. In this study rapid, scalable and robust in-air deposition method of ultrasonic spray pyrolysis (USP) has been applied to grow phase pure Sb_2S_3 thin films. Antimony chloride thiourea (SbTUCl) and antimony ethyl xanthate (SbEX) complex compounds were used as precursor materials [1,2]. Thermal analysis study (TG/DTA–EGA-MS) of precursors was performed to study the thermal decomposition reactions of precursor materials and determine the most suitable temperatures for Sb_2S_3 film deposition. Two-stage process where amorphous film with uniform thickness is grown by USP at temperatures around 200 ˚C followed by annealing at 260 ˚C in an inert atmosphere for 5 minutes results in polycrystalline single phase Sb_2S_3 as confirmed by XRD, Raman and EDX study. Using SbTUCl based precursor the optimal film deposition temperature was found to be 195 ˚C. In case SbEX precursor, amorphous Sb_2S_3 film could be grown even at lower temperature of 160 ˚C. When depositing the films by USP in air, measures to avoid oxidation during the film growth should be considered. It was shown that an excess of thioamides in spray solution is effective to depress the formation of oxide phase in films also confirmed by thermal analysis study. Thin film solar cells with structure TCO/TiO_2/Sb_2S_3/P3HT with all component layers prepared by solution methods in air showed conversion efficiency of 7.5% at AM1.5G and 18% at low illumination indoor conditions.

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The future of hydrogen fuel in aviation: economic analysis of current applications

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Keywords: hydrogen aircrafts, hydrogen fuel, economic analysis of hydrogen aircrafts, Data Envelopment Analysis (DEA)

Hydrogen fuel holds significant potential for sustainability in the aviation sector. This study conducts an economic analysis of five concept hydrogen powered aircraft models in relation to hydrogen fuel utilization. Using Data Envelopment Analysis (DEA), the evaluation determined that the fully efficient models in both technically and in terms of scale efficiency. Conversely, two concept models exhibit low scale efficiency and require optimization. The economic and operational feasibility of hydrogen fuel depends on factors such as infrastructure development, production costs, and regulatory policies. This study provides recommendations on technological and policy advancements necessary for the broader adoption of hydrogen in aviation.

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T07: Energy conversion and storage

Energy dissipation and thermal effect in cargo parachutes

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Keywords: operational reliability, numerical simulation, system performance, heat dissipation

During deployment of parachute systems, a significant portion of kinetic and potential energy is converted into thermal energy due to aerodynamic heating, fabric deformation and frictional interactions between suspension lines, canopy surfaces and the surrounding airflow. This energy conversion becomes particularly critical in high-speed deployments where intense aerodynamic forces and turbulent flow conditions contribute to localized temperature increases. The rapid inflation process, coupled with the interaction between the airflow and the fabric, generates frictional heat that can lead to the formation of burn marks on the parachute canopy. These thermal effects are influenced by factors such as deployment speed, atmospheric conditions and canopy material properties.

This study investigates the thermal effects of energy conversion during parachute deployment, focusing on the mechanisms responsible for heat generation and dissipation. Numerical simulations were performed using computational modelling platforms and analysis software to evaluate the intensity and spatial distribution of thermal energy. The findings of this research will improve the understanding of the thermal loads acting on parachutes and provide valuable insights into their impact on overall system performance and operational reliability.

Predicting solar cell temperature on soled surfaces: a study of dust thermophysical properties

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Keywords: machine learning, solar cell temperature, dust thermophysical characteristics, predictive modelling, random forests, financial losses

Soiling on solar photovoltaics leads to substantial losses in transmittance and increases in solar cell temperature, causing significant power losses. In addition, the accumulation of dust not only affect the transmittance of the solar cell but also increases the cell temperature. Increased temperatures have a significant negative impact on solar cell performance through a reduction in the energy generated. This study investigated the impact of dust particles on solar cell performance by examining their thermophysical properties, such as density, size, thermal conductivity, and specific heat. The study employed a systematic methodological approach, as illustrated in Fig. 1, to examine the effects of dust thermophysical properties on solar cell temperature and to develop a machine learning-based predictive model for solar cell temperature using random forests. Initially, the key thermophysical properties of dust, such as density, particle size, thermal conductivity, and specific heat capacity, were identified based on their relevance to the thermal behaviour of solar cells. An experimental design for the simulation runs was then developed to analyse the spectrum of these thermophysical properties and their impacts on solar cell temperature. Subsequently, ANSYS transient thermal analysis and Computational Fluid Dynamics (CFD) simulations were conducted using the Shear Stress Transport k-ω turbulence model and discrete phase model to analyse the effects of varying dust thermophysical characteristics. Exploratory data analysis identified significant variables for predictive modelling, utilising a random forest approach. The developed model achieved a coefficient of determination (R^2) of 0.973 and a mean absolute percentage error (MAPE) of 0.18°C. Energy simulations revealed an average annual energy loss of 22.18% due to soiling, with 4.5% linked to thermal effects, resulting in an annual financial loss of $1,907.26 for a 25 kWp system. These findings highlight the critical need for effective soiling management to improve solar panel efficiency and economic returns. The study emphasises the importance of accurately predicting soiled solar cell temperatures and illustrates that random forests are a viable method for temperature prediction.

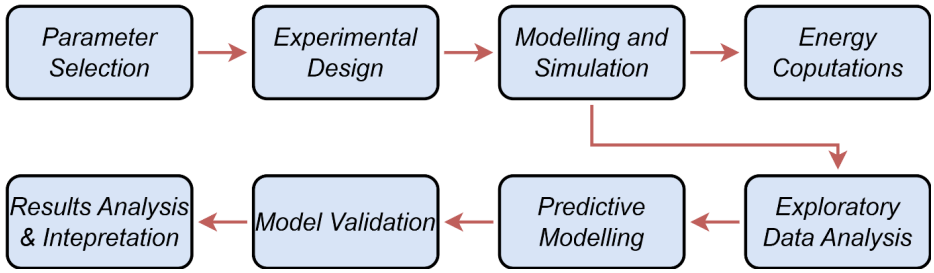

Figure 1 The research methodological approach

Aeronautics applications and design approaches of hybrid electric power train

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Keywords: digital twin, hybrid power train, electric motor and battery systems

This study explores the integration of components and numerical analyses based on technical specifications for the digital design of hybrid electric propulsion systems. The research focuses on the development of high-power-density electric motors that enable efficient power transmission. A digital design process has been implemented to create numerical models that accurately represent the performance characteristics of these motors under various operating conditions.

In addition to motor design, the study examines energy storage systems, with a particular emphasis on battery technologies used in hybrid propulsion configurations. The efficiency of these systems has been analyzed based on different battery chemistries, capacities, and energy management strategies. One of the key aspects investigated is the impact of increasing battery capacity on the overall flight range, assessing how energy storage improvements contribute to extended operational endurance.

Furthermore, the research evaluates the overall efficiency of hybrid propulsion systems by considering various factors such as power distribution, energy conversion losses, and system optimization techniques. The findings provide insights into how hybrid electric propulsion can enhance aircraft performance while balancing energy efficiency and power demands. The study ultimately aims to contribute to the advancement of hybrid aviation technology by offering a comprehensive digital framework for analyzing and optimizing hybrid propulsion architectures.

Detailed analysis responsibility in energy management of enterprises: a case study

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Keywords: enterprises, energy management, detailed audit, efficiency, sustainability

Energy management, one of the main sustainability indicators, requires a management responsibility that primarily considers, the current structure. Effective energy management includes monitoring, controlling and reducing energy consumption to increase efficiency and reduce costs, while businesses should manage the operational processes of energy users. For this purpose, detailed audits are directly required, including identifying energy-saving opportunities, evaluating current energy performance, and taking actionable actions. This study focuses on energy efficiency analyses and detailed audits, approached through a structured methodology. Opportunities related to electricity and natural gas usage in key energy-consuming areas were evaluated. Within this context, the energy efficiency savings potential of the Enterprise was found to be 4.69%. In the detailed analysis, five performance-improving projects (PAP) were proposed for the enterprise. These projects, which directly affect efficiency, collectively present a potential savings of 1,915,206 kWh per year, alongside an approximate reduction of 751 tons of CO2 emissions. The payback period for the improvements was found to average around 2.2 years. Additionally, three low-investment and no-investment opportunity suggestions were developed to enhance the company's energy efficiency further. These findings highlight significant potential for both cost savings and environmental benefits, providing a roadmap for more sustainable energy use within the enterprise.

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Brayton cycle design mathematical modeling and digital twin integration

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Keywords: digital twin, design, brayton cycle, gas turbine, modelling

Gas turbine engines form one of the critical subsystems of modern aviation systems, constituting a sophisticated engineering system based on the complex interaction of thermodynamic and aerodynamic principles. These engines, which fundamentally operate on the Brayton cycle, can be modified according to different operational requirements and utilized in various application areas. This study addresses the design of the Brayton cycle through mathematical modelling approaches. The dynamic behaviour and performance characteristics of the system- consisting of compressor, combustion chamber, and turbine components- are examined under parameters such as variable load conditions, atmospheric conditions, and altitude. In the modelling process, the thermodynamic properties of each component are analysed in detail, enabling the comparison of design and off-design operating conditions across the entire system. The integration of the developed model with digital twin technology significantly enhances the predictability of system performance. This approach eliminates the need for prototype production, providing substantial savings in both time and cost. This methodology, which particularly contributes to enhancing safety standards of critical importance in the aviation sector, represents a new paradigm in engineering design processes. The real-time simulation and analysis capabilities provided by digital twin technology have made it an indispensable tool for performance optimization and reliability analysis of gas turbine engines.

Thermal properties of shape-stabilized thermochromic phase change materials

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Keywords: phase change materials, thermochromism, shape-stabilization, thermal properties

Thermochromic phase change materials (TPCMs) are gaining increasing interest among scientists. These multifunctional materials are able not only to store thermal energy but also at the same time during the phase transition they can change their color. The main issue with these materials is liquid phase leakage during the melting process. The solution to this problem is using supporting materials to stabilize the shape of phase change materials. Aerogels are considered excellent support materials for effectively encasing PCMs, and preventing leakage, thanks to their strong capillary forces and surface tension. Leveraging their extremely low weight, exceptionally large surface area, and porosity, aerogels enable the highest possible PCMs loading, ensuring the maintenance of an exceptionally high energy storage density. Different types of aerogels such as polymer, carbon, cellulose, boron nitride, silica, graphene, and metal are used for PCMs shape stabilization [1-4].

This work aimed to study mainly the thermal properties of shape-stabilized thermochromic phase change materials. Fatty acids, fatty alcohols, and bromocresol purple were used as thermochromic system components. Two types of aerogels were used for shape stabilization. A thermogravimetry analysis was carried out to obtain data about the samples' thermal stability, which is crucial for materials subjected to temperature changes during their applications. The studies using the differential scanning calorimetry method allow for the comparison of two reversible processes occurring during the heating and cooling of the material: melting and crystallization. It is possible to compare the temperature ranges and latent heat values of these phase changes. Moreover, a DSC study was also performed in the so-called step mode (successive isothermal segments as a function of abruptly increasing temperature) to determine the amount of stored heat as a function of temperature. Additionally, the thermochromic properties were tested and positive results were obtained. This research showed that the tested materials have great potential as shape-stabilized thermochromic phase change materials for thermal energy storage.

Acknowledgments
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Thermal analysis methods in thermal energy storage applications

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Keywords: Thermal Energy Storage, sensitive, latent, thermochemical, thermal analysis methods, renewable energy

Thermal Energy Storage (TES) is an emerging and crucial technology for addressing global energy challenges. It is extremely relevant in the context of the ongoing transition to renewable energy sources. Renewable energies are intermittent by nature, the sun does not always shine or the wind blows, and it is a great challenge to accommodate consumption and production. Finding cost-effective, global and reliable storage solutions is essential to increase reliance on these renewable sources. TES offers a solution to mitigate power outages and increase energy access, contributing to the decarbonization of energy systems, reducing reliance on fossil fuels and supporting the shift toward sustainable, low-emission energy sources, which is vital in the fight against climate change. TES involves materials that can store heat and then release it when needed, making it an effective solution for balancing energy supply and demand. Thermal energy can be stored as sensitive, latent and thermochemical. Research is focused on improving the efficiency, capacity, and cost-effectiveness of TES technologies, which are critical for energy systems transitioning to more sustainable sources.
Thermal Analysis methods play a crucial role in thermal energy storage (TES) research by providing essential insights into the thermal properties, behaviour, and performance of materials used in TES systems. These methods provide information about how materials absorb, store, and release heat, which is fundamental for optimizing TES technologies. Thus, they are used for optimization of materials and cyclic conditions. In this lecture an overview of our experience in this field will be provided.

Acknowledgments
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Thermal decomposition of ordered and disordered LNMO

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Keywords: LNMO, Cobalt-free Cathodes, TGA, XRD

One of the hurdles in mass electric vehicle adoption is range anxiety with increased lithium-ion batteries energy densities being a solution to enlarge driving range. With this in mind, $LiNi_{0.5}Mn_{1.5}O_4$ (LNMO) is a potential cathode material that could increase the lithium-ion batteries energy density due to due to its high voltage plateau (4.7 V vs Li/Li^+). It is also lower in price and more ethical and environmentally friendly compared to other cathodes because it is Cobalt free and low in Nickel. Depending on the synthesis procedure, LNMO can have two crystal structures: ordered LNMO with a primitive cubic structure (P_4332) and disordered LNMO with a face-centered spinel structure (Fd-3m) where ordering refers to the distribution of the transition metal ions at the atomic positions. Our data sheds light onto the thermal decomposition behavior under air and argon of both the disordered and ordered by combining experimental data from thermogravimetric analysis (TGA), powder X-ray diffraction (pXRD), and high-temperature X-ray diffraction (HT-XRD). The data showed that, under air, ordered LNMO has a higher mass loss onset temperature in the TGA compared to the disordered LNMO. This mass loss is attributed to the formation of a Ni-rich rock salt structured phase and loss of oxygen and is reversible when cooling under air. The difference between the onset temperatures was elaborated further using HT-XRD. Under argon flow, however, no significant difference was found between both LNMOs with the mass loss not being reversible due to the absence of oxygen on cooling under argon. Powder-XRD was used to analyze the residual powder, and a model to explain the thermal decomposition of LNMO was concluded. The data obtained in this research will directly contribute to better fundamental understanding of LNMO getting us a step closer towards relieving range anxiety.

Thermal stability, thermochemical and thermophysical properties of lithium argyrodite solid electrolytes

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Keywords: solid-state battery, calorimetry, heat capacity, safety

Sulfide solid electrolytes exhibit the highest ionic conductivities (10^{-3}-10^{-2} S·cm^{-1}) of all solid electrolytes (SE) and are on par with liquid electrolytes.[1] Among SEs, lithium argyrodites $Li_{6-x}PS_{5-x}Cl_{1+x}$ are the most promising due to their decent cost efficiency.[1] As the thermal stability of solid-state batteries is a concern due to possible thermal runaway reactions and the potential formation of harmful gases,[2] understanding the thermal stability and other thermal properties of these materials is critical for the commercialization of solid-state batteries. However, the reported thermophysical properties of Li_6PS_5Cl are inconsistent in the literature. Some articles report its stability as high as 900 °C,[3] while in other investigations, the thermal decomposition occurs already in the 200–400 °C range.[4] Other compositions, such as $Li_{5.5}PS_{4.5}Cl_{1.5}$, are scarcely thermally investigated. Moreover, thermal properties besides thermal stability are often ignored for these materials.

We investigated the thermal stability of Li_6PS_5Cl from various sources using simultaneous thermogravimetry and differential thermal analysis coupled with mass-spectrometry (TG-DTA-MS) and simultaneous thermogravimetry and differential scanning calorimetry (TG-DSC). Investigations were carried out in inert (argon) or oxidative (synthetic air) atmospheres to evaluate the stability under differing environmental conditions. As found out in this work, the thermal stability of $Li_{6-x}PS_{5-x}Cl_{1+x}$ significantly depends on the synthesis method and manufacturer. We confirmed that in argon, Li_6PS_5Cl is stable up to 535 °C, while in air it starts to oxidize at 255 °C. Commercially acquired Li_6PS_5Cl is less stable, with the release of volatile species beginning in the worst-case scenario already at 140 °C (inert conditions).

We propose a straightforward method to evaluate sulfide SEs purity and stability: to analyze the sample by TG-DSC in an atmosphere switching from inert to oxidative after the sample is heated to an elevated temperature, namely 450 °C. This prevents instrument damage risks from potential corrosive material spilling at high temperatures and also providing the behavior of the sample in different atmospheres, inert and oxidative, in a single experiment.

Additionally, experimental thermodynamical data of specific heat capacities and enthalpies of combustion, and therefore enthalpy of formation, are collected for both SEs, Li_6PS_5Cl and $Li_{5.5}PS_{4.5}Cl_{1.5}$. The coefficient of thermal expansion was estimated for both solid electrolytes based on the unit cell parameter change in the temperature range 123-773 K. This allows the thermal modeling of solid-state batteries as well as strategic planning for their recycling.

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Thermal properties of carbonised citrus peels biomass infiltrated with sugar alcohols modified with graphene

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Keywords: phase change materials, thermal analysis, DSC, shape stabilization, long-term storage

Organic phase change materials (PCMs), especially sugar alcohols, have been of interest to scientists for many years. Particular interest arises from the high energy storage capacity [1,2]. Additionally, this organic material is unique because it has nearly twice the latent heat of fusion compared to other organic PCMs and is capable of working at higher temperatures [3]. The primary drawback of PCM lies in its solid-liquid phase transition, during which the volume changes, leading to a risk of leakage. Moreover, if nanoparticles are incorporated, sedimentation can occur, disrupting uniformity during the initial heating cycle [4].

In the literature, there are a few different ways to shape stabilization: using polysaccharides such as starch [5,6] or porous carbon materials from carbonization of selected fruit peels, for example, carbonized watermelon or orange peels [7,8].

The main goal of our research was to develop a shape-stabilized phase change material (PCM) for long-term energy storage. To achieve this, we prepared sugar-alcohol-based PCMs enhanced with graphene and infiltrated them into carbonized fruit peel modified with graphene. The properties of the resulting PCM composites were analysed using differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), scanning electron microscopy (SEM) and The Light Flash method (LFA). Furthermore, we calculated the percentage of PCM within the carbonized fruit biomass.

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Comprehensive analysis of turboprop engine performance across various flight conditions with exhaust gas temperature fluctuations using digital twin technology

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Keywords: turboprop engine, digital twin method, exhaust gas temperature, performance optimization, engine modeling

Turboprop engines are exposed to performance losses and thermal risks due to uncontrolled exhaust gas temperature (EGT) variations. This study provides a comprehensive analysis of exhaust gas temperatures of turboprop engines under different flight conditions. The main aim is to optimise exhaust gas temperatures in order to increase the efficiency of the engine during flight and to identify the most efficient flight conditions by evaluating the engine power based on exhaust gas temperature. To achieve this, the digital twin methodology was used to create a virtual engine model and a function to control the exhaust gas temperature. The digital twin approach allows real-time integration of data and continuous updating of the virtual model to ensure accurate monitoring of engine performance. The study examined exhaust gas temperatures under various variables, including flight altitudes, speeds and external atmospheric conditions, and assessed engine performance under different flight regimes. The results show that the function developed between the combustion chamber and the turbine effectively keeps the exhaust temperature within critical limits and avoids overheating. This is essential to optimising engine efficiency and to mitigate potential thermal damage. In conclusion, the study underlines the efficiency of Digital Twin technology in optimising the performance of turboprop engines and in controlling exhaust gas temperatures. In addition, the data obtained provide valuable insights for future flight optimisation studies, allowing for more accurate engine performance management and predictive control.

Lithium ion battery fire behavior and preventions

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Lithium ion batteries are essential in a broad range of strategic industries such as automotive, power grid, aerospace and consumer electronics. However, lithium ion battery thermal runaway arises from a series of undesirable side reactions accompanied by an uncontrolled temperature ascending, sometimes catastrophically accompanied by fire and explosion, which has impeded their further development. In this report, the thermal runaway mechanism is revealed from the heat generation, side reactions decoupling, thermodynamics, and thermal abuse test. Subsequently, the fire prevention strategies are proposed from the intrinsic safety, process safety, fire safety perspectives, of which the safe electrolyte, thermal management methods, fault diagnosis and fire suppression are considered to enable safe lithium ion battery. In the future, we appeal closer collaborations between the academia and industry to drive integration, improvements, harmonization and application of lithium ion safety across fields.

Thermodynamic and heat transfer modeling of ground source heat pump components for sustainable heating in cold climates: a case study of Kazakhstan

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Keywords: ground source heat pump, coefficient of performance, thermodynamic model, borehole heat exchanger, heat transfer simulation

This study presents a comprehensive experimental and theoretical investigation of ground source heat pump (GSHP) components for sustainable heating in cold climate conditions, with a focus on Kazakhstan. A three-dimensional numerical model was developed to simulate heat and mass transfer in the ground (modeled as a porous medium) and grout, coupled with one-dimensional conductive heat transfer through pipe walls and convective heat transfer within circulating fluid. The model was implemented using COMSOL Multiphysics and validated against thermal response test (TRT) data collected from a pilot installation in the Almaty region, where two 50-meter-deep boreholes were drilled. The TRT results showed strong agreement with both the simulation and analytical line-source models, with a root-mean-square deviation of 0.184 °C. Soil thermal conductivity and borehole thermal resistance were determined as λ_g = 2.35 W/m·K and R_b = 0.20 m·K/W, respectively.

The performance of various borehole heat exchanger (BHE) geometries was evaluated, including single and double U-tube, multi-tube, and spiral configurations. Among them, the spiral BHE demonstrated the highest heat extraction and enabled a reduction in required drilling depth by up to 34.6% compared to conventional configurations. Parametric studies revealed that higher grout thermal conductivity (0.5–3.3 W/m·K) and soil thermal conductivity (0.4–6.0 W/m·K) significantly improved heat extraction, while changes in pipe thermal conductivity and fluid flow rate beyond certain thresholds had negligible effects.

Additionally, a water-to-water GSHP system using refrigerant R134a was designed and tested for space heating. The predicted and measured coefficient of performance (COP) values agreed within 6.2%. The system's thermodynamic performance was further evaluated using alternative low-global-warming-potential refrigerants (R152a, R450A, R513A, R1234yf, and R1234ze). While R152a showed superior COP and low environmental impact, its high flammability limits practical use. Refrigerants R450A, R513A, R1234yf, and R1234ze were identified as promising substitutes, with only a 2–3% reduction in COP and significantly lower exergy destruction in comparison to R134a.

The developed model, experimental data, and findings provide a valuable framework for the design and optimization of GSHP systems in cold climates, contributing to the broader adoption of sustainable and energy-efficient heating technologies.

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T08: Exergy, experimental thermodynamics

Recovery of succinic acid through crystallization process: solubility and thermodynamics

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Keywords: solubility, succinic acid, glycerol, thermodynamic

This study evaluates the solubility and thermodynamic properties of succinic acid in four different glycerol-based solutions containing malic acid, sorbitol, and erythritol across various temperatures. The solubility of succinic acid was determined using synthetic in gravimetric methods. The experimental solubility data exhibited strong correlation with the van't Hoff model and demonstrated an increasing trend with rising temperature under all examined conditions. Thermodynamic parameter analysis indicated that the dissolution process of succinic acid is endothermic and entropy driven. The findings suggest that succinic acid is freely soluble in glycerol-based solutions under non-excess conditions.

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Enhancing atmospheric sustainability with vapour ad/ab-sorption systems

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Keywords: vapour adsorption and absorption, atmospheric water harvesting, thermochemical energy storage, desiccant-based dehumidification, AI-driven design optimization, sustainable climate control

Vapour adsorption and absorption systems are crucial for sustainable atmospheric management, enabling efficient moisture regulation, air purification, and waste heat recovery while facilitating freshwater extraction from the atmosphere. This study conducts a thermodynamic and exergetic analysis of desiccant-coated energy exchangers, liquid desiccant dehumidification systems, and thermochemical energy storage technologies, focusing on their role in atmospheric moisture harvesting and climate control. Adsorption/desorption kinetics of circular fin tube heat exchangers and hollow fiber membrane-based dehumidifiers are evaluated, considering moisture diffusivity, heat transfer coefficients, and structured packing effects for enhanced water capture efficiency. Computational modeling using Eulerian-Lagrangian multiphase simulations and discrete phase methods is applied to analyze moisture transport, condensation dynamics, and phase change behaviors in adsorption-driven water harvesting systems. AI-driven predictive optimization, integrating physics-informed neural networks, ANFIS, and KNN algorithms, enhances real-time control, optimizing energy efficiency and water yield. PCM-assisted thermochemical storage is examined for its effectiveness in sustaining continuous water extraction cycles. Comparative studies of liquid desiccant air conditioning, Ranque-Hilsch vortex tube cooling, and mobile thermochemical storage highlight their potential in atmospheric water harvesting, waste heat utilization, and decentralized cooling applications. The findings suggest that AI-enhanced optimization, coupled with advanced heat exchanger architectures and adaptive control, significantly improves the energy efficiency, scalability, and feasibility of vapour ad/ab-sorption systems for sustainable atmospheric applications, including clean water generation from ambient air.

Theoretical and experimental study on the usage of alternative A2L safety class refrigerants with low gwp in vertical type display cabinets

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Keywords: refrigerant, GWP, safety class, ISO 23953, A2L, COP

The current standard for the safety classification of refrigerants is ANSI/ASHRAE Standard 34-2019 Identification and Safety Classification of Refrigerants. There are two basic elements in the safety classification of refrigerants. The first is the toxicity effect; It is divided into two as A-slightly toxic and B-highly toxic. The second is the flammability effect; It was initially examined in three classes as 1-non-flammable, 2-flammable, 3-highly flammable. However, in later years, the 2-flammable class was divided into two and a new class, 2L-less flammable class, was added to this classification and is considered in four classes. Thus, there are now eight possible classifications: A1, A2L, A2, A3, B1, B2L, B2 and B3 [1]. Due to the climate change effect, the use of refrigerants such as R404A and R134A, which have high global warming potential, will be terminated. Today, refrigerants such as R290 and R1270, which are frequently used, have a high risk of fire and explosion due to their A3 safety class. The search for alternative refrigerants with low global warming potential and A2L safety class continues [2,3]. In this study, energy and exergy analyses were performed for R454C, R455A, R1234yf, R1234ze(E), which are refrigerants with low global warming potential and A2L safety class and can be used instead of R404A, R290 and R1270 gases. In addition, within the scope of this study, tests were performed on refrigerated display cabinets using R1270 and R454C according to the ISO 23953 standard. Thermodynamic analyses were carried out at various evaporation temperatures for a constant condensing temperature of 30 °C and at various condensation temperatures for a constant evaporation temperature of -5 °C. In the analyses, the highest STK value was obtained as 4.91 with R1234ze(E) refrigerant, while the lowest COP value was obtained as 3.51 when R455A was used. The highest specific cooling capacity values were obtained as 314.1 kJ/kg with R1270 refrigerant, while the lowest capacity was obtained as 129.6 kJ/kg when R1234yf refrigerant was used. When we compare these refrigerants in terms of exergy efficiency; R290, R1270 and R1234ze(E) refrigerants have an exergy efficiency of 43%, while R1234yf and R404A refrigerants are close to these values and have efficiencies of 42% and 40%, respectively. R454C and R455A fluids have the lowest values and are 33% and 31%, respectively. Although R1234ze(E) fluid is thermodynamically good, its evaporation pressure is low (-5°C 1.79 bar). Therefore, low pressure problems may be encountered in low temperature applications. In the experimental tests, when R1270 fluid was used, the lowest product temperature was measured as -0.41°C, while the highest product temperature was measured as 3.78°C. In the test conducted using R454C fluid, the lowest product temperature was measured as -0.81°C, while the highest product temperature was measured as 3.59°C. Both tests were conducted according to the test chamber climate class 3 (25°C/60%) in the ISO_23953 standard, and the test package temperatures met the M0 (-1/+4) conditions.

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Comparative performance assessments of CO_2 refrigeration cycles under subcritical and transcritical operating conditions

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Keywords: refrigeration, natural refrigerant, CO_2, carbondioksit, transcritical

The extensive use of synthetic refrigerants, such as hydrochlorofluorocarbons (HCFCs), hydrofluorocarbons (HFCs), and chlorofluorocarbons (CFCs), in the refrigeration and air conditioning industries over the past few decades is a major factor contributing to climate change and an increase in the average global temperature [1]. As a result, CO_2 has been reexamined as a feasible substitute for sustainable refrigeration systems in light of the growing restriction of hydrofluorocarbons (HFCs) and hydrochlorofluorocarbons (HCFCs) because of their high global warming potential (GWP) [2]. Carbon dioxide (CO2 or R744) is a natural working fluid with zero ozone depletion potential (ODP) and unit GWP. Because of its superior thermodynamic qualities, CO_2 refrigeration systems can be used in air conditioning, heat pumps, and commercial refrigeration. The high working pressures of CO_2 systems, however, provide a challenge that calls for a robust system design and materials that can endure these circumstances. Transcritical CO_2 refrigeration cycles have gained significant attention as an efficient and environmentally friendly alternative to traditional refrigerants [3]. Unlike conventional refrigeration cycles, which operate entirely in the subcritical phase, transcritical cycles utilize CO_2 in both supercritical and subcritical states, making them particularly useful in high-temperature environments. A transcritical CO_2 refrigeration system operates at pressures above the critical point of CO_2 (73.8 bar, 31.1°C), where the refrigerant does not condense in a conventional manner. Instead of a condenser, a gas cooler is used to reject heat. The efficiency of these cycles is highly dependent on factors such as gas cooler outlet temperature and high-side pressure optimization. To overcome efficiency drawbacks associated with high operating pressures, various modifications have been introduced. One such advancement is the ejector expansion transcritical cycle, where an ejector replaces the conventional expansion valve to recover expansion work, thus enhancing efficiency. Another improvement includes the integration of mechanical subcooling, which helps lower the gas cooler outlet temperature, thereby improving system performance. Transcritical CO_2 refrigeration cycles represent a promising solution for high-efficiency, environmentally sustainable cooling systems. With continued advancements in technology, these systems are expected to become more widespread, particularly in commercial and industrial applications. A refrigerator using a CO_2 cycle in indoor environments may need to operate in both transcritical and subcritical conditions under real operating conditions. Therefore, it must be designed to operate in both cycle states. In this study, the comparative thermodynamic performance analyses of the CO_2 cooling systems operating under subcritical and transcritical conditions were carried out for different working conditions. The variations of the system performance were examined and compared under subcritical and transcritical working conditions.

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Tewi analysis and environmental impacts evaluation of the refrigerants used in the refrigerated display cabinets

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Keywords: TEWI, GWP, safety class, ISO 23953, A2L

The refrigeration sector is responsible for 7.8% of the world's greenhouse gas emissions, of which 37% are direct emissions from refrigerant leakage and 63% are indirect emissions from electricity consumed. In order to minimize the environmental damage of refrigerants, studies on new generation refrigerants are important. TEWI (Total Equivalent Warming Impact) analysis is a generalized calculation method that calculates the CO_2 emissions caused by a refrigeration device during its lifetime [1]. In this analysis, direct emissions from refrigerant leakage and indirect emissions from energy consumption are calculated. In refrigerant selection, indirect emissions from energy consumption are often overlooked because of the focus on the global warming potential of the fluids. Due to the climate change effect, the use of refrigerants such as R404A and R134A, which have high global warming potential, will be terminated. Today, refrigerants such as R290 and R1270, which are frequently used, have a high risk of fire and explosion due to their A3 safety class. The search for alternative refrigerants with low global warming potential and A2L safety class continues [2,3]. Within the scope of present study, a comparative analysis is performed for the environmental effects of R404A, R454A, R455A, R1234yf, R1234ze(E) gases, which are mainly used in refrigerated display cabinets. The energy performances of the refrigerated display cabinet by employing the R1270, R454C, R744(class3) and R744(class0) refrigerants were measured according to ISO23953 standard. In the present performed analysis, the lowest CO_2 emission was obtained as 24.327 tn_{CO2} when R1270 fluid was used. For R454C, R744(class3), R744(class0), R404A, R455A, R1234yf, R1234ze(E) fluids, 36.599, 70.080, 31.650, 39.620, 39.464, 29.507, 28.677 tn_{CO2} values were obtained respectively. The highest emission value was obtained at class3 operating conditions of R744 gas due to high energy consumption. Energy consumption and emission values decreased by half when the R744 gas-fired cabinet was operated under class0 conditions. The main reason for this is that R744 gas works much more efficiently in sub-critical form. Although R455A has a lower global warming potential than R404A, it emits more CO_2 emissions during its lifetime due to its inefficiency. In R404A fluid, direct emissions take a significant value of 21%. Among the A2L fluids evaluated in this study, the lowest emission values were obtained when R1234yf and R1234ze(E) fluids were used.

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T09: Fuels, biofuels

Exergy analysis of biomass gasification systems: a pathway to enhanced energy recovery and process sustainability

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Keywords: biomass, energy analysis, exergy analysis, gasification

The rising demand for renewable energy necessitates the development of efficient biomass conversion processes. Among these, biomass gasification is a versatile technology for producing syngas, a valuable intermediate for biofuels and chemicals. This study investigates the thermodynamic performance of biomass gasification systems using exergy analysis to identify sources of irreversibility and optimize energy recovery. Key system components, including the reactor, heat exchangers, and syngas cleanup units, are evaluated to determine exergy destruction and improve overall process efficiency. The influence of operating conditions, such as gasifying agents, temperature, and pressure, on exergy efficiency is thoroughly analyzed. Comparative assessments of different reactor configurations—fixed-bed, fluidized-bed, and entrained-flow systems—are conducted to highlight the thermodynamic advantages of each design. The findings provide actionable insights for minimizing energy losses and enhancing the sustainability of biomass gasification processes, contributing to the broader goals of carbon-neutral energy systems and circular economy initiatives.

Optimization of non-recyclable medical plastics using pyrolysis for high-yield biofuel production

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Keywords: medical waste, pyrolysis, latex gloves, waste management, circular economy

Medical waste has significantly increased leading to serious health and environmental issues such as disease spread and contamination of air, water, and soil. Among these wastes, latex gloves (LG) classified as thermosetting polymers are non-recyclable through conventional means, unlike thermoplastics such as polyethylene (PE), polypropylene (PP), and others. This study investigated the use of pyrolysis as an effective thermal conversion method to valorize LG waste into valuable products: pyrolysis oil, char, and gas. The process was conducted in a fixed batch reactor with the primary objectives of maximizing oil yield and enhancing the fraction of high-value compounds in the oil. Key process parameters, including temperature, heating rate, retention time, and particle size were optimized. Characterization techniques included CHNS elemental analysis for LG and char, FTIR spectroscopy for functional group identification, and GC-MS for pyrolysis oil composition. Under optimal conditions (300 °C, 12 °C/min heating rate, 30 min retention time, 0.5–2 cm particle size), the process yielded 61 ± 1.5 wt.% oil, 22.67 ± 1.5 wt.% char, and 16.00 ± 1.5 wt.% gas. The oil was found to contain 91.57% limonene—a high-value compound with applications as a biofuel additive, and in pharmaceuticals, food, and cosmetics. This work demonstrated a sustainable and economically viable approach to managing non-recyclable medical waste, supporting circular economy initiatives through zero-waste conversion to high-value products.

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Thermochemical valorization of tomato plant residues: characterization of the pyrolysis process through the coupling of TGA-based kinetic analyses and pilot-scale auger reactor tests

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Keywords: tomato plant residue, pyrolysis, thermogravimetric analysis, kinetic modeling, auger reactor

The tomato is one of the most widely cultivated vegetables and fruits in Canada. In 2024, more than 548,107 tons of tomatoes were produced across a total area of 6,153 hectares [1]. However, tomato cultivation generates vast quantities of biomass waste (approximately 15 t ha^{-1} y^{-1} for greenhouse systems [2]), including green residues such as stems, leaves, and branches. Despite their abundance, these residues remain largely underutilized, with disposal methods such as landfilling contributing to greenhouse gas emissions and other environmental concerns. In this context, pyrolysis offers a promising approach to address waste management challenges while simultaneously generating a wide variety of biochemicals and high-value biofuels. The pyrolysis of biomass typically yields three main products, each with distinct applications: biochar, bio-oil, and syngas. Biochar, a carbon-rich solid, is widely used for soil amendments, carbon sequestration, and wastewater treatment due to its high surface area and adsorption properties. Bio-oil, a complex mixture of organic compounds and water, can be upgraded into alternative fuels for boilers and engine applications. Syngas, primarily composed of CO, CO_2, H_2, and CH_4, is suitable for combustion in boilers or gas turbines and can also be used as a feedstock for chemical synthesis. Despite the growing interest in biomass valorization, research on the pyrolysis of tomato plant residues remains limited, particularly at the pilot scale. As a result, the influence of key operational parameters on product distribution and composition remains insufficiently understood. To address this gap, the present work investigates the pyrolysis of tomato plant residues (TPR), primarily composed of stems and leaves, using both a thermogravimetric analyzer and a pilot-scale auger reactor. First, thermogravimetric analyses (TGA) were performed to evaluate kinetic parameters accounting for the pyrolysis behavior of TPR. Measurements were carried out using 4 heating rates: 5, 10, 15, and 30 K/min. The results obtained were then processed by means of 3 isoconversional methods (namely, Kissinger–Akahira–Sunose (KAS), Flynn-Wall-Ozawa (FWO), and Friedman). Based on the obtained rate constant parameters, the variation of the

fuel conversion degree as a function of the temperature was simulated while considering different reaction mechanisms commonly employed in the literature, including order-based, diffusion, geometrical, nucleation, and power law models. As highlights, the results obtained using the three isoconversional approaches closely matched the TGA experimental data. The agreement between simulated and measured data was found to be higher in the case of the Friedman model, followed by the KAS and FWO. In a second step, a series of experiments were conducted in an auger reactor by setting two reaction temperatures (400 and 600°C) and two solid residence times (75 and 125 s) to assess the influence of these key operating parameters on the properties of obtained products. The elemental composition and mineral contents of the collected biochar were characterized ex situ, while the syngas composition, including CO, CO_2, H_2, CH_4, and C_nH_m fractions, was monitored online during the tests. Regarding the bio-oils, their elemental composition, water content, pH, density, and lower heating value were determined. Furthermore, Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) was also used to analyze and gain insights into the oligomeric composition of the bio-oils. Results indicate that the highest bio-oil yield (25.2%) was achieved at 600°C and for a solid residence time of 125 s. FT-ICR MS analysis revealed that the bio-oil obtained at 600°C contained a higher proportion of light compounds as compared to its counterpart produced at 400°C. Additionally, the bio-oil produced with the higher temperature exhibited a greater presence of oxygen-poor and non-oxygenated species, along with a higher relative concentration of saturated species.

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Follow-up study on valorization of carrot pomace via pretreatment and hydrothermal liquefaction - characterization and thermal analysis of produced biocrude

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Keywords: carrot pomace, waste, HTL, hydrolysis, extraction, biocrude, pyrolysis, thermochemical conversion, biofuels

Poland is the second-largest carrot producer in the European Union, with an annual production of 842,000 tons, according to Eurostat data from 2023 [1]. Carrots are widely processed into various products, including juices, mousses, and concentrates. During this processing, the main byproduct is carrot pomace, which is characterized by high moisture content and low stability. Depending on the juice extraction method, between 0.35 and 0.55 kg of pomace is generated per 1 kg of raw carrots [2]. Given the significant quantities of carrot pomace generated in the processing industry, developing efficient valorization pathways is essential. Rich in various saccharides, carrot pomace can serve as a substrate for the production of bunch of chemicals, especially so-called platform chemicals Additionally, it can be converted into high-energy-density materials such as biocrude, biochar, or biogas, or used as a precursor for value-added chemicals obtained through thermochemical processes. Hydrothermal liquefaction (HTL), a promising method for carrot pomace utilization, converts biomass into biocrude and solid hydrochar. This study builds upon previous research optimizing sugar recovery through pretreatment and subsequent HTL conversion. In this work, particular attention is given to the characterization of biocrude obtained via HTL from carrot pomace subjected to different pretreatment strategies, namely: (i) no pretreatment, (ii) hot water extraction, and (iii) a two-step pretreatment involving hot water extraction followed by acid hydrolysis. The HTL process was conducted at 315°C for 10 minutes, as these conditions were found to be optimal for biocrude production. To assess their properties, the obtained biocrude were characterized using elemental analysis (CHNSO), gas chromatography–mass spectrometry (GC-MS), gel permeation chromatography (GPC), and Fourier transform infrared spectroscopy (FT-IR), which provided insights into their composition, molecular weight distribution, and functional groups. Furthermore, the biocrude underwent additional thermochemical conversion through pyrolysis, with the evolved volatiles analyzed using microscale techniques, including pyrolysis–gas chromatography/mass spectrometry (Py-GC-MS) and pyrolysis–Fourier transform infrared spectroscopy (Py-FT-IR). The results indicated that hot water extraction led to an increase in biocrude yield compared to untreated material, although with a slight decrease in its calorific value. Conversely, the application of additional acid hydrolysis resulted in biocrude with improved combustion properties and a narrower molecular weight distribution. The pretreatment type significantly influenced the molecular weight range of biocrude compounds, with hot water extraction leading to a slight increase in average molecular weights, while acid hydrolysis resulted in a reduction and a more uni-

form distribution of molecular masses. Moreover, the combination of hot water extraction and acid hydrolysis effectively reduced the oxygen content in the HTL-derived biocrude and contributed to an increase in higher heating value (HHV). These improvements enhance the suitability of biocrude for fuel applications, demonstrating that controlled pretreatment strategies can be used to optimize both yield and quality.

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Application of digital twin technology for comprehensive analysis of turboprop engine performance, combustion, and emissions across varied fuel types

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Keywords: fuel types, turboprop engine, performance optimization, engine modeling, digital twin method, emissions

The examination and analysis of the various types of jet fuel in gas turbine engines are of great importance for ensuring optimal performance and safety in the aviation sector. The main purpose of this study is to compare emission values of different fuel types used in turboprop engines and to identify the most efficient engine operating power. In this study, the digital twin method was used for performance optimization. By creating a virtual engine model, main performance parameters such as the pressure ratio, engine airflow, gas generator speed, exhaust gas temperature, and output torque can be kept at optimal levels without exceeding critical values. The accuracy and reliability of the model shall be supported by the quality of the data sets from the physical system and by the ongoing process of verification of the model. Simulation was performed by testing different fuel types in this virtual environment. The findings showed that the digital twin approach is an effective method for analysing engine performance. The virtual model makes it possible to identify issues quickly, boost productivity, and save money and time. The simulations carried out comprehensively evaluated the effects of different fuels on engine power and emission values were compared. The findings show which fuel type provides the best results in terms of environmental sustainability and fuel efficiency.

Properties of spinel-based oxygen carriers for chemical looping combustion examined by using thermogravimetric analysis

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Keywords: CLC, TGA analysis, oxygen carriers, spinels

Chemical looping combustion (CLC) is a new, low-emission technology of fuel combustion, that might be applied for reducing of greenhouse gas emissions due to simplification of CO_2 capture. In the CLC process, all oxygen required for the combustion process is delivered by an oxygen carrier (OC), therefore fumes are not diluted with atmospheric nitrogen and are predominantly composed of carbon dioxide and water vapor. A significant challenge to the commercialization of CLC is the degradation of the oxygen carrier during repeated reduction-oxidation cycles, emphasizing the necessity for an OC to maintain its properties during operation in a CLC reactor. One of the potential candidates for oxygen carriers are spinel-based ferrites, a class of mechanically durable materials that exhibit high oxygen transfer capacity. Some of them are also capable of releasing gaseous oxygen in a reaction for a changes of temperature and O_2 partial pressure in the reaction environment in a process named Chemical Looping with Oxygen Uncoupling (CLOU). In the following research, thermogravimetric analysis of selected ferrite spinel-based oxygen carriers was shown.
The performance of the oxygen carriers was evaluated through a series of experiments involving the combustion of solid and gaseous fuels (syngas). The experiments were conducted on thermogravimetric equipment. Multiple repeated cycles of reduction and oxidation with specific fuels were performed to mirror the conditions encountered in a CLC reactor.

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Comparative analysis of diesel and wco blends in terms of engine emissions, efficiency, and fuel consumption

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Keywords: Waste Cooking Oil (WCO), diesel engine emissions, engine performance optimization, alternative fuels

The present study examines the impact of incorporating waste cooking oil (WCO) into diesel fuel on engine emissions, efficiency, and fuel consumption under varying operational conditions. Three types of fuels were analyzed: pure Diesel, DieselWCO20 (20% WCO blended with Diesel), and DieselWCO40 (40% WCO blend). The study was conducted on an internal combustion engine that was subjected to a variety of operating conditions, including varying engine speeds, loads, and air-fuel equivalency ratios (Lambda). The study aimed to assess the impact of using WCO-blended fuels on major pollutants like CO, CO_2, HC, NO, and PN, as well as key performance indicators like BTE and BSFC. The significance of differences among the three fuel types regarding emissions, efficiency, and fuel consumption was assessed through a traditional statistical approach, specifically the non-parametric Kruskal-Wallis test. The findings revealed statistically significant differences, especially in CO and PN emissions, suggesting that these factors are markedly affected by the fuel composition. Fuel variation was studied using advanced modeling methods, and the correlation between engine operating parameters and outcome variables (emissions, efficiency, and consumption) was simulated. These comprised artificial neural networks (ANNs) and limited regression analysis. The developed mathematical models allowed exact prediction of engine behavior across a multidimensional space of input variables. Contour plots were produced utilizing these models to illustrate the influence of operational parameters on each output variable, thereby facilitating the discernment of optimal engine operating conditions for each fuel type. In addition to the single parameter study, composite indicators were developed to assess the overall performance and environmental impact of each fuel. The amalgamation of various efficiency criteria and emissions into a singular score facilitates a comprehensive comparison of different fuel types. The findings suggest that while WCO-blended fuels may elevate certain emissions, including carbon monoxide and particulate number, they concurrently present benefits in various areas, notably a reduced reliance on fossil fuels and poten-

tial enhancements in efficiency under specific operational circumstances. The study provides a comprehensive framework for assessing alternative fuels using a combination of statistical analysis, machine learning models, and performance visualization. It demonstrates that blending diesel fuel with waste cooking oil not only has measurable effects on engine performance and emissions but also offers a viable path toward more sustainable fuel usage in internal combustion engines. Engine parameters have to be painstakingly fine-tuned to balance performance with environmental effect. Including spent heating oil into conventional diesel fuels can assist to lower contaminants and increase the value of waste. The findings may serve as a thorough evaluation for researchers, legislators, and corporate tycoons engaged in creating ecologically beneficial fuel substitutes.

Catalytic hydrodeoxygenation of bio-oil produced from co-pyrolysis of biomass and plastic waste

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Keywords: biomass, plastic, co-pyrolysis, bio-oil, red-mud, upgardation

The rising energy demand and the decreasing availability of fossil fuels have driven the pursuit of renewable fuel sources from biomass and plastic waste [1]. However, biofuel production faces challenges due to the high free fatty acid content in waste lipids [2]. To improve fuel quality, oxygen removal is essential. This study explores the catalytic hydrodeoxygenation of bio-oil derived from the co-pyrolysis of *Mesua ferrea* L. (Nahar, a non-edible oilseed) and PET plastic. Operating parameters, including temperature and biomass-to-plastic ratio, were optimized, revealing a maximum bio-yield of 35 wt% at 600 ℃ with a 2:1 biomass-to-plastic ratio. Qualitative analysis of the co-pyrolyzed oil showed that fatty and carboxylic acids (~55%) were the dominant components, necessitating further upgrading for potential applications. In the upgrading process, red mud (RM), an alkaline waste from alumina production via the Bayer process [3], was used as a support material for mono-metallic (Ni) and bi-metallic (Ni-Co) catalysts. These catalysts were characterized using BET, FESEM-EDX, FETEM, XRD, ICP-MS, and XPS. They were then applied in the hydrodeoxygenation (HDO) of co-pyrolytic oil, with the Ni-Co/RM catalyst achieving the highest organic liquid yield (72%) while minimizing coke formation and maximizing hydrocarbon yield (80%). Using mono- and bi-metallic catalysts at a reaction temperature of 300 ℃, the HDO process effectively reduced the acid content of raw bio-oil (~55%) while significantly enhancing hydrocarbon yield (80%). The primary reaction pathways observed were hydrodeoxygenation (HDO) and decarboxylation (DCO).

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Performance and emission characteristics of ternary blends of fish oil biodiesel in the dual-fuel systems using single and split injection strategy

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Keywords: biodiesel, fish oil, ternary blends, dual-fuel engine, combustion, emissions, performance, split injection

The escalating global demand for sustainable energy solutions and the environmental concerns associated with conventional fossil fuels have intensified the search for renewable alternatives. Among these, biodiesel derived from waste or non-edible fish processing residues presents a promising avenue. This study investigates the performance, combustion, and emission characteristics of ternary blends of fish oil biodiesel, diesel, and ethanol in a gasoline dual-fuel engine. The experimental analysis was conducted using a single-cylinder, four-stroke, water-cooled diesel engine operated at a constant speed of 1500 rpm under varying load conditions. The results demonstrate that ternary blends exhibit improved combustion characteristics, with higher peak pressures and heat release rates compared to diesel, indicating more efficient energy conversion. Specifically, peak cylinder pressures reached 74.2 bar in single injection mode and 71.5 bar in split injection mode, compared to 76.2 bar for diesel. The rate of pressure rise (RoPR) was notably higher for diesel at 5.2 bar/°CA in single injection mode, whereas the ternary blends exhibited a more controlled combustion process, with RoPR values of 4.8 bar/°CA and 4.2 bar/°CA in single and split injection modes, respectively, reducing mechanical stresses on engine components. Heat release rate (HRR) analysis revealed that ternary blends achieved peak HRR values of 62.3 J/°CA in single injection mode and 58.7 J/°CA in split injection mode, indicating superior energy conversion efficiency. In terms of engine performance, ternary blends showed significant improvements in brake thermal efficiency (BTE) and lower brake specific fuel consumption (BSFC), particularly in split injection mode. The BTE for ternary blends reached a maximum of 32.4% in split injection mode, compared to 30.1% for diesel. The BSFC was reduced to 0.27 kg/kWh under split injection, highlighting enhanced fuel economy and reduced fuel wastage. Additionally, brake power (BP) was higher for ternary blends, particularly in single injection mode, further confirming their superior combustion efficiency. Emission analysis revealed that ternary blends exhibit lower carbon monoxide (CO), unburned hydrocarbons (HC), and nitrogen oxides (NO_x) emissions compared to diesel. Split injection mode effectively reduced NO_x emissions by 15% by moderating peak combustion temperatures, while CO and HC emissions were consistently lower due to the oxygenated nature of biodiesel and ethanol, promoting more complete combustion. Although CO_2 emissions were slightly higher for ternary blends due to their lower carbon-to-hydrogen ratio, split injection optimized the combustion process, ensuring more efficient CO_2 production. The cumulative heat release (CHR) analysis further

confirmed that ternary blends provided a more efficient combustion process, contributing to enhanced overall engine performance. These findings underscore the potential of ternary blends of fish oil biodiesel, diesel, and ethanol as a cleaner and more efficient alternative to conventional diesel in gasoline dual-fuel engines.

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Hydrogen economy and thermal management: challenges, opportunities, and future perspectives

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Keywords: hydrogen economy, thermal management, aviation, sustainable aviation, carbon emissions

The hydrogen economy plays a crucial role in global energy transition and sustainability goals. The need to reduce carbon emissions has accelerated the search for alternative fuels in energy-intensive sectors such as aviation. In this context, hydrogen presents significant potential as a clean and efficient energy source. However, there are operational, financial, and technical obstacles to its broad use in aviation. In particular, storage and transportation at cryogenic temperatures pose critical thermal management issues.

This study examines the impact of the hydrogen economy on the aviation sector and explores the challenges of thermal management. It evaluates existing technologies and strategies for hydrogen utilization, assessing their contribution to sustainable energy transition. By providing a conceptual framework, the study aims to enhance the understanding of hydrogen integration in aviation. The findings highlight the technical and managerial challenges of hydrogen adoption in aviation and summarize recent developments addressing these issues. The authors recommend that future research should focus on optimizing hydrogen storage systems and developing cost-effective production methods.

Computational fluid dynamics in hydrogen internal combustion engines: a review of current applications, challenges, and future directions

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Keywords: hydrogen, internal combustion engines, hydrogen combustion modelling, sustainable energy, computational fluid dynamics

Hydrogen internal combustion engines (H2ICEs) have emerged as a promising carbon-neutral solution amid the global shift toward decarbonization, leveraging hydrogen's high energy density and zero CO_2 emissions. However, their adoption faces challenges due to hydrogen's unique combustion properties, including high flame speed [1], low ignition energy [2], and wide flammability range, alongside risks of nitrogen oxides emissions [3], pre-ignition, and material incompatibility. Computational Fluid Dynamics (CFD) has become indispensable in addressing these challenges, offering high-fidelity insights into fuel-air mixture formation, spray dispersion, and combustion dynamics. Advanced CFD techniques, such as turbulence-chemistry interaction models and flame propagation simulations, enable detailed analysis of hydrogen's autoignition behavior and lean-burn combustion regimes. 3D transient simulations resolve under-expanded hydrogen jet interactions with in-cylinder charge motion, guiding injector layout optimization to enhance mixture homogeneity [4]. Large Eddy Simulation (LES), Detached-Eddy Simulation (DES), and Reynolds-Averaged Navier-Stokes (RANS) approaches are widely employed to model turbulent flows, though challenges persist in accurately capturing laminar flame speed (LFS) and ignition delay time (IDT) for hydrogen combustion. This study reviews the techniques in conducting CFD simulations for H2ICE, highlighting its potential to bridge the gap between experimental research and industrial deployment while charting a roadmap for next-generation, sustainable engine technologies. Remarkable studies will be critically discussed to elucidate key challenges in applying CFD to H2ICE simulations. Future research directions will also be proposed to provide insights into developing more comprehensive and realistic CFD for H2ICE design analysis. By addressing current limitations and prioritizing model validation, CFD can accelerate the transition to hydrogen-powered transportation, positioning H2ICEs as a viable pillar of the decarbonized energy landscape.

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T11: Heat transfer

Comparative heat transfer enhancement analysis in Cu-H_2O, Al_2O_3-H_2O and Cu-Al_2O_3-H_2O: computational approach

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Keywords: hybrid nanofluid, heat transfer analysis, finite difference method

In recent years, researchers have increasingly concentrated on the enhancement of heat transfer due to its extensive applications across various industries. To improve the heat transfer rate of base fluids, the incorporation of nanoparticles and hybrid nanoparticles has emerged as a compelling area of study. This talk will focus on the comparative analysis of heat transfer in the flow of nanofluids, specifically Copper- Water and Aluminum Oxide-Water, alongside a hybrid nanofluid, Copper-Aluminum Oxide-Water, over stretchable permeable sheets. The analysis will consider nanofluids in saturated porous media described by Darcy's law, accounting for the effects of thermal radiation and viscous dissipation in the energy equation. The flow problem will be formulated as a system of coupled partial differential equations (PDEs). By employing suitable dimensionless variables, the system will be transformed into a dimensionless form. The resulting dimensionless PDEs will be solved computationally using the finite difference scheme. The outcomes will be presented and analyzed through graphs and tables, discussing the impacts of flow variables—including Reynolds number, porosity parameter, nanoparticle shapes, nanoparticle fraction, suction/injection parameter, thermal radiation, and Eckert number—on skin friction, velocity, Nusselt number, and temperature.

Biomimetic liquid-cooled heat sink for efficient thermal management applications

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Keywords: liquid cooling, thermal management, heat sink, cooling technologies

The rapid advancements in artificial intelligence and the increasing demand for compact electronic systems have posed significant challenges in designing efficient and effective thermal management solutions. This study presents the design and investigation of a novel liquid-cooled heat sink that minimises flow resistance while maximising effective surface area for enhanced heat dissipation. Inspired by the fish respiratory system, particularly the fluid flow mechanism, and considering the shape of tuna and black ghost knife fish, an innovative pin-fin configuration has been introduced, as shown in Fig. 1. A comparative analysis was conducted between the proposed heat sink and a conventional straight-channel heat sink. The novel design features a hybrid pin-fin arrangement consisting of airfoil-shaped pin-fins surrounded by corrugated curvilinear pin-fins, strategically positioned on the heat sink surface. To evaluate the hydrothermal performance, an experimental test rig was fabricated and validated [1]. The experiments were performed at varying flow rates ranging from 200 mL/min to 450 mL/min while maintaining a constant heating power of 150 W. The results demonstrated that the Airfoil Integrated Corrugated Curvilinear Pin-Fin (AICCPF) heat sink achieved a twofold enhancement in Nusselt number compared to the conventional straight-channel heat sink. At the highest flow rate, the Nusselt number increased from 7.60 to 15.5, indicating an approximately 103% improvement in heat transfer efficiency, Fig. 1. Additionally, the pressure drop was found to increase by 37.5%, while the average wall temperature was reduced by up to 4.52°C. The findings of this study underscore the potential of the proposed biomimetic heat sink design for next-generation thermal management applications, particularly in high-performance electronics and AI-driven systems. The integration of AICCPF offers an optimised balance between heat dissipation and fluid flow resistance, making it a promising solution for advanced cooling technologies.

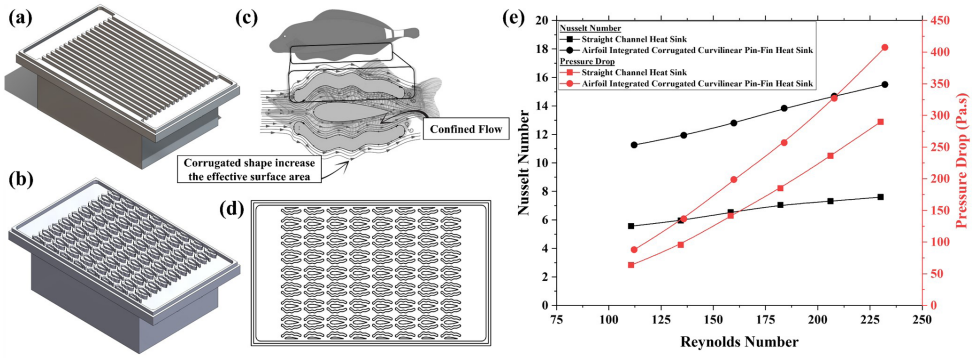

Figure 1. (a) Straight channel, (b) Airfoil-integrated corrugated curvilinear pin-fin heat sink, (c) Biomimetic heat sink design inspiration, (d) Pin-fin arrangement, and (e) Comparison of Nusselt number and pressure drop.

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Thermal energy optimization for interacting fluid with solid structure in novel configuration with finite element simulations

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Pervasive applications of thermal energy transmission due to interaction of non-Newtonian materials with cylinders placed in confined configurations has been found in diversified engineering mechanisms. For instance, hydropower generation, electronic cooling system, HVAC, thermal exchangers and many more. So, the motive of current study is to analyze thermal energy transport in non-Newtonian (Power law) fluid filled in trapezoidal channel with symmetric cavities and containing cylinder of circular shape. Both forced and free convections are investigated at different regions of domain. Equations are developed after incorporation of rheological and associated features of momentum and temperature distributions. Formulation showing coupling between equations is changed into dimensionless version after employment of variables. Numerical simulations are performed by executing finite element simulations through COMSOL software. Initially, in pre-processing distribution of domain into hybrid elements composed of triangular and rectangular shapes is done and linear and quadratic polynomials for pressure, velocity along with temperature profiles are used to estimate behavior of variables on nodes. Grid independence test is performed to certify independence of simulations of mesh size. Results are drawn for wide range of parameters and their impact of associated distributions is exclusively analyzed. Drag and lift coefficients along with averaged heat flux coefficient which play vital role in such studies are enumerated against various parameters. Visualization of cutlines to ensure behavior of velocity and temperature profiles at different locations of channel are also displayed.

Simulation of the pcm encapsulation effect on natural convection of a horizontally placed li-ion battery using the lattice boltzmann method

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Keywords: Thermal lattice Boltzmann method, lithium-ion battery, phase change material, battery thermal management system

With the increasing adoption of electric vehicles (EVs), ensuring the safety of lithium-ion batteries has become a critical concern. To address this, the Thermal lattice Boltzmann Method (TLBM) incorporating a phase change material (PCM) model has been further developed and implemented on a GPU, significantly reducing computational costs. This study investigates the effectiveness of passive air cooling enhanced by PCM in maintaining battery temperatures within an optimal operating range. Four PCM vessel shapes, i.e. circular, square, hexagonal, and a proposed modified design, are analyzed to evaluate their impact on cooling efficiency. Results reveal that the circular-shaped PCM vessel achieves the highest heat absorption efficiency in enclosed systems, reducing battery temperature by 3.3°C compared to the square-shaped vessel. In ventilated configurations, the square-shaped vessel exhibits superior heat dissipation, lowering temperature by 3.4°C, while the hexagonal shape ensures better temperature uniformity. Additionally, a modified vessel shape enhances airflow balance and PCM distribution, further improving thermal regulation with a 1.5°C reduction relative to the square-shaped design. These findings highlight the importance of optimizing PCM vessel geometry for effective battery thermal management under different cooling conditions.

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Numerical study of Stefan problem with two moving domains and variable thermal properties

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Keywords: Stefan problem, two moving domains, size-dependent permeability, Vieta-Luca polynomials

This study presents a mathematical model for a melting problem in a two-phase region which involves variable thermophysical properties to investigate the temperature distribution and mass density in both regions. The considered model contains two moving domains. The numerical solution to the problem is acquired by employing a numerical method based on the operational matrix of Vieta-Luca polynomials. The accuracy of the presented method is validated through a comparison with the exact solution achieved in a particular case and it is identified that current results are sufficiently near to them. The consequences of different dimensionless parameters on temperature and moving curves are presented graphically. This study's findings provide ways to accelerate the speed of phase transition with minimal energy absorption of particles during the phase change process.

The exact solution for Stefan problem is not always achievable. Hence, numerical techniques [1], [2] are being used to solve such problems. In this article, we examined a highly nonlinear model describing the drying process. The main purpose of this study is to discuss the effect of size-dependent permeability in the freeze-drying process.

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A numerical investigation on bioconvection flow considering growth rate term

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Keywords: bioconvection flow, oxytactic bacteria, growth rate

In this study, natural bioconvection flow is investigated considering the logistic growth of bacteria. The problem is numerically simulated in a square cavity filled with oxytactic bacteria in the presence of oxygen concentration.

The time dependent governing dimensionless equations are solved by radial basis function method in space derivatives and backward Euler method in time derivatives. The numerical results are not only observed in different dimensionless parameters but also examined in distinct values of growth rate of bacteria as well as consumption of oxygen. The growth rate term is added to the bacteria density equation while the consumption of oxygen is also set as dependent on bacteria density. In case of Peclet number less than or equal to one, the rise in growth rate term results in a little bit rise in the average bacteria density, Nusselt and Sherwood numbers. The significant behaviour is noted by the increase in consumption rate of oxygen with which the average Nusselt number decreases in the system while the Sherwood number rises, and the average bacteria density declines.

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Identification of temperature distribution during the welding process

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Keywords: contact heat conduction, heat generation, inverse method, control volume method, diagnostic system

When bodies of different temperatures are in mechanical contact, heat is transferred between them by various mechanisms, including heat conduction. Temperature changes in bodies affect mechanical, thermal and other processes. In many technological processes, such as sliding friction, machining or welding, the contact surface of the bodies is subjected to intensive heating. Therefore, the analysis of the temperature distribution, including the contact surface, is important. Often, due to technical limitations, the measuring element of the temperature sensor cannot be located directly on the interface. An example is welding, where temperatures in the interface can destroy the temperature sensor or monitoring the temperatures of fast abrading friction elements. In such situations, inverse heat conduction problems (IHCP) are often convenient to determine the distribution of the contact temperatures and heat fluxes, using measuring elements installed at a safe distance from the interface. Many publications deal with IHCP in various fields of science, as reported by Beck et al. [1], or Chen et al. [2] but few of them are devoted to the study of heat conduction taking into account the contact resistance and the analysis of heat fluxes for a moving heat source. Nosko [3] developed an algorithm for the solution based on an inverse parametric optimisation method, using a first-order thermocouple model with an impulse response function describing the heat partition and contact heat transfer. Wen-Lih [4] estimated the unknown time-dependent frictional heat flux at the interface of two semi-spaces with the assumption of the unknown heat generation. Ökten [5] developed method to determine the melt pool geometry and temperature distribution in the heat-affected zone while Zhang et al. [6] use an inverse method to determine the thermal conductivity of copper oxide.

The proposed inverse method is based on the control volume method and can be used for simple shapes such as a pipe or plate. It allows to identify the temperature distribution even for multilayer elements, taking into account the contact resistance. The method allows for the inclusion of temperature-dependent material properties. The entire analysis area is divided into control volumes for which heat balance equations are solved. First, the equations for the layer near the surface with temperature sensors are solved. In this way, we obtain temperature transients on the next layer. Then, in a stepwise manner, the equations for all layers are solved, obtaining transients temperature for all nodes. The method also allows for determining the heat transfer coefficient on the unknown boundary condition and the heat flux density on the contact surfaces.

The proposed identification method is verified by comparing the obtained solutions with the results from the direct method. The developed algorithm can be used during monitoring of precise welding processes. It can contribute to the improvement of welded joints.

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Preliminary study of textile structures with regard to their photonic radiative cooling properties

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Keywords: IR responsive textile, textile photonic structures, radiative cooling, biomimetic approach

In the context of climate change, this project deals with the development of radiative cooling textiles to face heat waves [1]. The literature proposes different radiative cooling approaches: multilayer (e. g. oxide based multilayer structure), periodic structure, random structure[2], bio inspired (butterfly wings) [3]. This project focus on the development of biomimetic photonic textile structures based only on speciality fibres and advanced fibrous structures excluding the use of non-environmentally friendly chemicals. Particular interest is taken to structural photonic structures such as the Saharan silver ant (cataglyphis bombycina). In this particular case the ant's hairs are covering its body and their morphology provides 75% of IR reflection in the wavelength range [0.8-1.4 µm] [4]. The aim of this preliminary study is to identify the intrinsic parameters of basic textiles that influence the quality of infrared radiation reflection. The intrinsic parameters considered are the colour lightness, the fibre nature and morphology, the textile porosity and air permeability, as well as the textile fabrication technology

The selection of textiles fabrics is composed of 4 nonwoven fabrics, 2 wovens fabrics, 2 knitted fabrics, 5 fabrics based on PET fibres, 2 based on cotton fibres, 1 with flax fibres, 5 white fabrics, 1 grey, 1 black and 1 with raw natural colour. These fabrics include fibres diameter in the range 7.5 to 30 micrometres. An integrating sphere spectrometer is used to measure the reflectivity in the [1-1.4 µm] range. A spectrophotometer is used to determine the fabric colour lightness (L coefficient). Some temperature measurements in a pseudo in situ situation of the textile fabric under a IR lamp are carried out. The IR lamp is positioned on top of a textile fabric, producing 1kW/m² of heat flow (closed to the energy produced by the sun). Temperature sensors are positioned close to the top of the textile (T_1), close to the bottom (T_2) and further down (T_3) to measure the protective effect of the fabric. The surface temperature of the textile above (T_4) and below (T_5) is also measured using a thermal camera.

As expected, the colour lightness is a relevant influencing factor. The lighter the colour the higher the reflection. Accordingly, the reflection is exponentially increasing with the lightness. The first results so show that the textile fabrication technology (woven, knitted or nonwoven fabric) seems to have no influence on the averaged reflection. Concerning the fibre type, the fabric made of cotton fibres seems to be a little more reflecting than polyester fabric. The bicomponent pie-wedge fibre provides higher IR reflexion, in comparison to traditional . The pie-wedge fibre after splitting shows similarities in the fibre morphology of the silver ant hair reaching 65% of IR reflectance. The in-situ measurement demonstrates that the temperatures measured below the textile (T_5 and T_2) are decreasing with an increasing IR reflectivity. Moreover, textile fabric thickness and porosity influence the temperature difference between

the two textiles surfaces (T_4-T_5). In conclusion, this preliminary study has enabled us to identify the most relevant intrinsic parameters and to highlight certain avenues for research into the development of bio-inspired photonic textile structures.

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Design, manufacture and characterisation of cryogenic test facility for low-noise amplifiers

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Keywords: cryogenic test facility, low-noise amplifier, vacuum system, radio astronomy, cryostat

This study presents the development and characterization of a dedicated cryogenic test facility housing low-noise amplifiers (LNAs) for radio astronomy applications. Effectively reducing the noise temperature of the LNAs through a suitable thermal and vacuum system is pivotal for enhancing the sensitivity of radio telescopes, which is crucial for advancing astronomical discoveries. A review was conducted on the different cooling and vacuum pumping methods currently available to determine the most suitable options. A test system was designed and manufactured according to design specifications, with standard cleaning procedures applied to machined components. Mathematical models were formulated to describe the thermal and pressure characteristics of the cryostat. Temperature and vacuum experiments were conducted aimed at achieving minimal temperatures and establishing optimal vacuum conditions for efficient thermal management and preservation of electrical component integrity. The first and second stages achieved minimum temperatures of 11 K and 38 K, respectively, reasonably close to the calculated values of 13 K and 42 K. The utilization of a heat shield to optimize cooling conditions resulted in a modest reduction in the second-stage temperature and extended the cooldown time for both stages by 30 minutes. Vacuum tests conducted on the pumping station, manifold, and the cryostat yielded pressure readings of 4×10^{-7} mbar, 1.5×10^{-5} mbar, and 2.5×10^{-5} mbar, respectively. Pressure decay results indicate that outgassing is the primary contributor to the gas load, surpassing O-ring permeation. The extensive use of stainless steel in the cryostat and manifold resulted in high concentrations of hydrogen gas within the vacuum. This understanding underscores the effectiveness of vacuum baking as the most efficient method to improve vacuum conditions, ultimately decreasing the requirement for vacuum maintenance and extending observation times. This research offers practical insights into the design and maintenance of cryogenic systems, which reduce initialization and maintenance time, thus optimizing operational efficiency.

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Thermal performance of a new standalone solar dryer for drying apple slices

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Keywords: portable solar dryer, apple slices, drying characteristics, thermal performance

Improving the shelf-life of fruits and vegetables, extending their drying time, and preserving their nutritional content remains an enormous challenge in Africa. In response to this problem, a light, stand-alone, low-cost, portable solar dryer was fabricated and investigated experimentally using two consecutive 8-hour tests on two days, and a continuous overnight 32-hour test. The dryer requires minimal technical maintenance and operates in sunny and cloudy conditions. The drying chamber consisted of four metallic trays and 2 DC fans powered by 12 V batteries charged by a 50 W PV panel to remove moisture continuously inside the chamber. The average solar radiation affecting the drying chamber and thermal profiles were 718 W m-2 and 706 W m-2 on day 1 and day 2 respectively, whereas an average of 377 W m-2 was obtained for the continuous 32-hour test. A maximum temperature of 63.5 °C was recorded in the top tray during day 2 of the 8-hour test, whereas a maximum temperature of 66.5 °C in the top tray was obtained during the 32-hour continuous test. An increase in the relative humidity was observed at the beginning of the first drying day, and it reached the minimum value of 16 % at the end of the successive and continuous drying tests. A minimum moisture level of 15 % was achieved in the 16-hour tests on the top tray, while a minimum moisture value of 14 % was obtained for the 32-hour test. The drying efficiencies for the 8-hour tests were 12.2% and 1.6% for day 1 and day 2, respectively, while the drying efficiency for the 32-hour test was 8.4 %.

Human mental search (hms) algorithm and adaptive network-based fuzzy inference system (anfis) to model the heat transfer in a heat exchanger equipped with a new type of self-rotating tube insert

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Keywords: adaptive network-based fuzzy inference system, heat transfer enhancement, human mental search, hybrid model, self-rotating tube insert, thermal-hydraulic performance ratio

Using tube inserts have been known as an efficient technique to improve heat transfer (HT) in heat exchangers. Prediction of the HT rate is highly important for this equipment. In this investigation, the human mental search (HMS) algorithm is integrated with the adaptive network-based fuzzy inference system (ANFIS), and a novel hybrid model is constructed. The proposed hybrid model is used to predict the experimental values obtained, i.e., Nusselt Number (Nu), friction coefficient (f), as well as thermal-hydraulic performance ratio (η), in a heat exchanger equipped with tube inserts. The designed insert includes different self-rotating modules. The rotating insert is offered to cause a secondary sweeping flow on the inner side of the tube. The thermal-hydraulic performance ratio considers both favorable HT enhancement and undesired pressure drop (PD) created by this type of insert. The decision factors are the number of inserts ($0 \leq N \leq 30$), tank temperature ($40 \leq T \leq 50$), velocity inlet ($5 \leq U \leq 15$), and Prandtl Number ($0.7138 \leq Pr \leq 0.7186$). The highest value of the thermal-hydraulic performance ratio was found 1.45 in conditions of the Prandle Number of 0.715, water temperature of 40 °C, insert number of 30 and, velocity inlet of 5 m/s (Reynolds Number of 6000), which confirms that the inserts perform better at lower velocities.The proposed hybrid model is trained, tested, and finally evaluated by the experimental results.

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3-D CFD analysis of a correlation between nusselt numbers and thermal boundary layer from a heated horizontal cylinder rotating in air: from laminar to turbulent flow

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Keywords: rotating cylinder, heat convection, CFD, laminar, turbulence, full-field analysis

A 3-D computational fluid dynamics model is developed to reproduce the results of previous experiments and to investigate the correlation between Nusselt numbers and convection heat transfer phenomena surrounding an isothermal rotating cylinder. The simulation is conducted in a quiescent air domain and a fixed Grashof number of 2.32×10^8 for a horizontal cylinder placed in air with rotational speeds ranging from 2.43 to 103.22 RPM. The effects of buoyancy induced flows and the rotational Reynolds number on convective heat transfer characteristics are investigated. At low Re_r, buoyancy-driven Rayleigh–Bénard convection dominates, forming vertically extended thermal plumes obstructing heat convection on the upper side of the cylinder, leading to lower Nusselt number in these regions. As Re_r increases, rotational effects intensify, altering flow dynamics and progressively enhancing heat transfer in the turbulent regime, where cylinder-driven flow fully dominates convection. At very high Re_r, the merging of flow plumes with the cylinder surface thickens the thermal boundary layer, suppressing heat transfer efficiency. The circumferential Nusselt number distribution further highlights that plume formation lowers Nusselt number on the descending side, while heat transfer is enhanced along the axial direction toward the cylinder ends, where the thermal boundary layer thickness gradually decreases.

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Novel approach to identify the effective heating region of closed-loop pulsating heat pipe using four-step method

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Keywords: Closed-Loop Pulsating Heat Pipe, effective heating region, thermal performance, four-step method

A Closed-Loop Pulsating Heat Pipe (CLPHP) is a two-phase passive device that operates without an external power supply for cooling. It has gained significant attention for its highly effective heat transfer capabilities, making it a promising solution for various cooling applications [1]. Most of the existing literature focuses on evaluating thermal capacity by considering the entire heating zone and using average thermal parameter values for CLPHP. However, there is limited research on identifying the most efficient heat dissipation zone or investigating dry-out conditions and critical limits, which significantly impact thermal design, safety, and scalability for industry-ready applications. For the first time, this study proposes a novel approach called the Four-Step Method to identify the effective heating region and determine the critical limits in CLPHP. The experimental work on CLPHP is performed using deionized (DI) water with a filling ratio (FR) of 60% and various heat inputs (80W, 100W, and 120W). The CLPHP is oriented vertically with heat supplied at the bottom. The Four-Step Method utilizes the Python library PyPulseHeatPipe for the investigation [1]. This Python library enables advanced data analysis, visualization of data, and identification of effective heating region. The major objectives of this method are to identify the effective heating region, measure effective pulsation, determine critical limits, dry out precautions, initiate the force convection, and enhance governance and safety of CLPHP for industry-ready usage. Figures 1 and 2 show the variation of condenser temperature with evaporator temperature and pressure with evaporator temperature for FR of 60% under various heat inputs, respectively. When compared to the subcritical point (effective heating starts) at 80W, the heat transfer enhancement reaches a maximum of approximately 31.94% at 120W and a minimum of about 21.67% at 100W. Similarly, compared to the critical point (effective heating ends) at 80W, the maximum thermal enhancement is approximately 36.30% at 120W, while the minimum is around 34.22% at 100W. The Four-Step Method for CLPHP can enhance thermal design, maintain stable operation under high heat inputs, and be applied for various filling ratios, inclination and title angles, working fluids, and industrial applications.

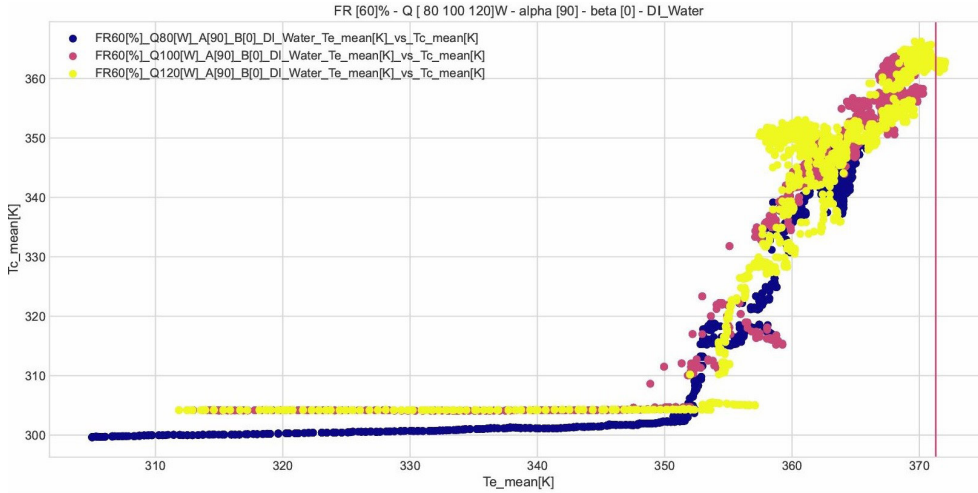

Figure 1: Variation of condenser temperature with evaporator temperature

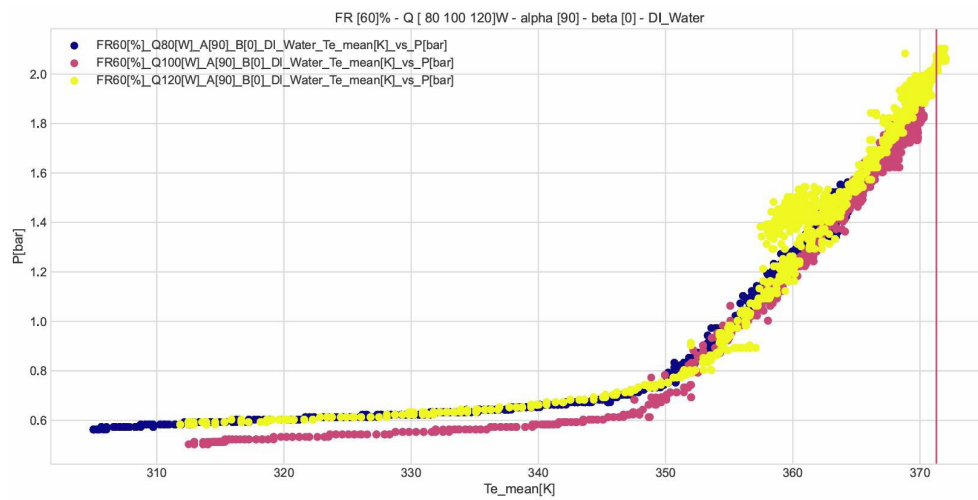

Figure 2: Variation of pressure with evaporator temperature

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Numerical investigation on bioconvection flow in the presence of two concentrations

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Keywords: magnetotactic bacteria, RBF method, oxygen concentration, Fe concentration

In this study, natural bioconvection flow in the presence of magnetotactic bacteria is numerically investigated bacteria in a square cavity involving water and two concentrations. The concentrations are considered as oxygen and iron (Fe) concentrations. The time independent governing dimensionless equations in stream function-vorticity form are numerically solved by using radial basis function collocation method. The numerical results are observed in different Rayleigh (Ra), bioconvection Rayleigh (Rb), Peclet (Pe), Lewis (Le_1, Le_2) numbers and the buoyancy ratio parameters. The average Nusselt and Sherwood numbers along the heated wall, and the average number of bacteria all around the cavity are calculated as well as plotted contours. In case of two concentrations, the diffusivity of bacteria is assumed to be equal to one of the concentration diffusivity. Firstly, the diffusivity of bacteria is assumed to be equal to the diffusivity of oxygen concentration. The average Nusselt number as a measurement of convective heat transfer increases with the rise in Ra, Rb, Pe and Le_2 numbers. The elevation in buoyancy ratio parameters affects average Nusselt number, average Sherwood number of Fe and average density of bacteria inversely. The average Sherwood number of Fe as an indicator for the convective mass transfer of Fe remarkably decreases as Le1 increases in this first assumption. On the other side, the second assumption for the equality of diffusivity of bacteria to the diffusivity of Fe reduced the convective heat transfer significantly as Le_2 rises.

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Lithium-ion battery thermal management system for regional temperature extremes in himalayan climates: a CFD analysis

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Keywords: thermal management, lithium-ion battery, discharge rates, Reynolds number, CFD, inline arrangement and staggered arrangement

The thermal management of lithium-ion batteries is very essential particularly in regions such as Kashmir in the Himalayas where the temperature variations range from -4°C to 24°C to ensure the safety, efficiency and longevity of the electric vehicle battery packs. The present study primarily investigates the effects of seasonal ambient temperatures in Kashmir (winter: 4°C, spring/autumn: 15°C, summer: 22°C) with varying discharge rates (2C and 3C) and Reynolds numbers (4,000-16,000) on the thermal performance of the lithium-ion battery packs. A Finite Element Method (FEM) based COMSOL Multi-physics software is used to numerically investigate the effect of varying discharge rates, ambient temperatures and Reynolds numbers in staggered and inline battery configurations. Maximum Temperature (T_{max}), maximum temperature difference (ΔT) and Cooling Performance Index (CPI) are used as thermal performance assessment parameters. A relative performance assessment between the two battery configurations reveals that the staggered battery arrangement depicts better cooling efficiency at higher discharge rates and higher inlet temperatures. This better thermal performance in staggered arrangement can be attributed to better air flow distribution ensuring lower T_{max} and ΔT values. On the other hand, the inline battery configuration depicts inferior cooling characteristics as far as T_{max} and ΔT values are concerned in comparison to staggered battery configuration. The battery thermal management systems were optimised to keep the battery pack within permissible temperature ranges throughout the year, ensuring dependable operation of electric vehicles and energy storage systems in Kashmir's severe climatic conditions.

Would heat sources and human thermal plumes affect indoor airflow and particle dynamics in healthcare facilities? A state-of-the-art review

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Keywords: indoor heat sources, thermal plumes, airflow dynamics, particle dispersion, thermal analysis

Heat sources and human thermal plumes within indoor environments significantly shape airflow patterns and particle dynamics in healthcare facilities, directly impacting infection control measures and overall thermal comfort. Healthcare facilities are designed to limit the spread of airborne pathogens through controlled ventilation and particle management. However, heat generated by medical equipment, lighting, and human occupants disrupts airflow patterns, affecting the dispersion and deposition of infectious particles. Additionally, elevated air temperature and relative humidity can promote bacterial growth [1], potentially increasing healthcare-associated infection (HAI) rates. This review critically examines existing literature on the impact of heat sources and thermal plumes on airflow behaviour, emphasizing their interaction with particle transport and ventilation efficiency. It explores the fundamental mechanisms by which heat sources produce thermal plumes and how these plumes interact with mechanical ventilation systems. The analysis incorporates both experimental findings and computational fluid dynamics (CFD) simulations to illustrate the effects of temperature gradients on particle trajectories. Particular focus is given to human-induced thermal plumes, driven by metabolic heat generation (ranging from 58 W/m² to 116 W/m²) [2]. These plumes interact with mechanical ventilation, influencing the dispersion patterns of infectious aerosols. Notably, human thermal plumes significantly deflect exhaled airflow with velocities around 1 m/s, whereas exhalation velocities exceeding 1.5 m/s experience minimal deflection [3]. The review highlights how localized heat sources, such as medical equipment (110 W/m²) and surgical lamps (255 W/m²), alter velocity profiles and temperature fields, thereby affecting airborne particle transport [4]. Also, various ventilation strategies, such as displacement ventilation, vertically downward ventilation, and personalized airflow delivery systems, are assessed for their efficacy in mitigating the impact of thermal plumes. One study demonstrated that temperature-controlled personalized airflow (21–24°C) could extend the clean zone around burn patients by up to 82%, enhancing recovery and reducing particle deposition [5]. The influence of heat sources on airflow patterns is further examined,

particularly the interaction between supply air jets, human body plumes, and shear flows. When the downward air jet and the human thermal plume are of comparable strength, complex flow patterns emerge, with thermal plume velocities reaching up to 0.275 m/s [6]. This comprehensive review underscores the critical impact of thermal influences on optimizing ventilation strategies to reduce the risk of airborne infections in healthcare facilities.

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Simulation study on enhanced refrigeration system performance through the integrated use of microtube evaporator and expander

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Keywords: refrigeration cycle, microtubes, expander, coefficient of performance

This simulation study introduces an innovative approach to enhance the performance of a refrigeration cycle through the integration of a microtube evaporator and an expander. Using the Engineering Equation Solver (EES) software, a refrigeration cycle with a nominal capacity of 14 kW was modeled to assess its coefficient of performance (COP) and power consumption. The analysis examines changes in condensing and evaporation temperatures, along with the inner diameter of microtubes, for the refrigerants R454C and R454B, which are characterized by low ozone depletion potential and low global warming potential. Four configurations were evaluated: the base cycle, a cycle with an expander, a cycle with a microtube evaporator, and a cycle incorporating both an expander and a microtube evaporator. Condensing and evaporation temperatures were varied between 30–45°C and -10–10°C, respectively, while the microtube inner diameter ranged from 0.3 to 5.2 mm. Results indicate that R454B achieves a COP 13.8% higher than R454C, demonstrating superior energy efficiency. The expander reduces power consumption by an average of 27.1% compared to the base cycle. The combined cycle configuration achieves a 52% increase in COP relative to the microtube evaporator cycle alone. Power consumption is minimized with smaller microtube diameters, showing an 11.1% reduction as the inner diameter decreases from 5.2 mm to 0.3 mm in the combined cycle. Overall, the combined configuration proves to be the most efficient, reducing power consumption by approximately 32% and outperforming the expander, microtube evaporator, and base configurations, respectively.

Acknowledgments
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Evaluation on comprehensive performance of drying system of spent resin integrated with a heat pump cycle by waste heat recovery

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Keywords: drying, heat pump, spent resin; waste heat recovery, thermodynamic and economic analysis, aspen plus

Cation exchange resins (CERs) are cross-linked polymers with functional groups. Through the cation exchange process, CERs are commonly applied in many fields, such as water softening, metallic compounds recovery, and the treatment of contaminated water. However, the exceptional water absorption and retention capacities of CERs would trigger substantial economic burdens on transportation, regeneration, and disposal processes of spent resins. Drying is a critical technology for reducing moisture levels of spent resins, thereby enhancing the treatment efficiency and ensuring the long-term safety and stability of disposal processes. The heat pump is a feasible approach to realize the waste heat recovery, which has the potential to be applied in energy efficiency improvement of the drying systems. In current work, a novel drying system integrated with a heat pump was proposed for spent resin drying to tackle high energy consumption and heat loss in drying. The hot air with high temperature and low humidity from the condenser was fed into the drying chamber to dry the spent resin. The emitted air with high humidity and waste heat from the drying chamber flowed into the evaporator, where the moist air was cooled. Subsequently, the cooled and dehumidified air returned to the condenser to be heated to high temperature. A thermodynamic model was developed to evaluate the system's performance. The comprehensive performance including environmental impact, energy, exergy and economy availability of the integrated system based on Aspen Plus software was evaluated, in terms of refrigerants (R123a, R245fa, R600, R290, R1234ze(E), R1233zd(E)), flow rate of the refrigerants, evaporation and condensation temperature. The optimal capital investment and operational costs of the drying system were also determined. A reduction in CO_2 emissions appeared through the use of the optimal refrigerant, by life cycle climate performance (LCCP). The data could provide some guidance for designing and operation drying systems of spent resin with highlighted performance.

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Experimental-numerical determination of correlations for nusselt numbers on the hot and cold medium sides of a tube-in-tube coil heat exchanger

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Keywords: tube-in-tube coil heat exchanger, heat transfer correlations, experimental testing, numerical method, least squares method

This study introduces a novel approach for simultaneously determining correlations for Nusselt numbers in a tube-in-tube coil heat exchanger. The system operates with hot water flowing through the inner tube while cold water moves through the annular gap. The experimental research focused on a coil heat exchanger functioning as either an evaporator or a condenser in a heat pump system. Measurements were taken to record the temperatures of both the hot and cold fluids at the inlet and outlet, along with their respective mass flow rates. A computerized data acquisition system facilitated data collection, ensuring that only steady-state operation measurements were selected for analysis. Through extensive experimental trials, four unknown coefficients—two for each side of the central tube wall—were identified using the least squares method. These coefficients were determined by minimizing the sum of squared differences between the measured and computed outlet temperatures of the hot and cold fluids. The mathematical expressions for the Nusselt numbers on the inner and outer surfaces of the central tube were derived based on momentum and energy conservation equations for turbulent fluid flow in a straight tube. Additionally, 95% confidence intervals were established for the four coefficients.

The developed correlations for the Nusselt number in both the inner tube and annular gap are applicable in engineering design and performance analysis.

T12: Inorganic materials

The growth, optical, and thermal characterization of CdBeSeTe quaternary mixed crystals using photothermal methods

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Keywords: thermal characterisation, CdBeSeTe semiconductor crystals, piezoelectric photothermal spectroscopy, photopyroelectric technique (PPE)

Cadmium telluride-based materials are among the most promising semiconductors for X-ray and γ-ray detector applications. By adjusting the composition of mixed crystals, it is possible to modify their electronic properties, lattice parameters, and band gap energy, thereby tuning their optical response across the visible and UV spectrum.

In this study, we investigate cadmium beryllium selenide telluride ($Cd_{0.99}Be_{0.01}Se_xTe_{1-x}$) quaternary crystals with selenium content (x) varying from 0 to 0.2. The samples were grown from the melt using the vertical Bridgman Stockbarger method and characterized using two photothermal methods, each associated with a different nature of generating the photothermal signal. The piezoelectric photothermal spectroscopy (PPS) enables measurements in the front and reverse configurations and applies a piezoelectric detector to measure the photothermal signal. It is sensitive to the surface preparation of the sample [1] and enables the determination of the optical properties of the materials. The photopyroelectric technique (PPA) is a contact method that directly measures heat oscillations [2] and allows for the determination of thermal properties. The analysis focused on evaluating thermal diffusivity, effusivity, and conductivity which are crucial parameters for understanding heat transport mechanisms in semiconductors. Transmittance measurements were conducted to evaluate the optical properties of the material, particularly the band gap variation with selenium content. The results indicate a decrease in thermal diffusivity and effusivity with increasing selenium content, suggesting that selenium incorporation influences heat conduction in the material.

The results presented in this work contribute to the fundamental understanding of CdBeSeTe as a new material. The interplay between its optical and thermal properties, influenced by selenium incorporation, highlights its potential in infrared detectors, thermoelectric devices, and other optoelectronic applications. Given the novelty of this quaternary compound, these findings serve as a foundation for further research and optimization.

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Revisiting assumptions: thermal behavior of ammonium nitrate systems with additives commonly considered as stabilizers

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Keywords: ammonium nitrate, exothermic decomposition inhibitors, thermal analysis

Ammonium nitrate (AN) remains a compound of high industrial relevance-and equally high risk [1, 2]. Due to numerous documented explosions caused by systems containing AN, the topic of its stability in the presence of various additives has been extensively studied with the use of thermal analysis [3-5]. Despite decades of research into its thermal stability, many substances continue to be classified as decomposition inhibitors based primarily on open-system assessments that emphasize the endothermic decomposition process [6-8]. This study systematically re-evaluates that classification under closed-system conditions using differential thermal analysis coupled with thermogravimetry and mass spectrometry (DTA-TG-MS). Ten additives, including various phosphates, carbonates, nitrogen-containing organics, and a reference promoter (ammonium chloride), were tested across three mass ratios (4:1, 9:1, 49:1) in binary mixtures with ammonium nitrate. Samples were heated to a temperature of 450°C in air atmosphere.

The findings challenge the assumption that stabilizing effects are universal across thermal regimes. For multiple systems, additive presence led to earlier onset of exothermic decomposition, greater heat release, or multi-stage reaction pathways not evident in open-system studies. Additional DSC-TG-MS measurements of selected mixtures under open crucible conditions illustrate how misleading conclusions may arise from incomplete testing setups.

These results emphasize the critical need to reframe how stabilizers are evaluated in ammonium nitrate systems, particularly in light of practical storage and confinement conditions. This work aims to refine experimental approaches and highlight inconsistencies in how thermal stability is currently assessed in the literature.

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Influence of temperature on the synthesis of acid geopolymer

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Keywords: phosphate geopolymer, thermal curing, MAS NMR spectroscopy, isothermal calorimetry

Acid-based geopolymers is emerging group of materials produced by mixing of an aluminosilicate precursor and phosphoric acid. Their advantage, compared to conventional binders, is superior thermal and chemical stability, which determine their potential application to thermally and chemically resilient coatings, thermally-insulating foams or 3D-manufacturing [1]. One of the principal factors, which influences the properties of prepared acid geopolymer is curing temperature – scholars have used room temperature, but more frequently 60 to 80 °C for 1 or more days [2]. Temperature is apparently influencing the kinetics of geopolymeration process which consists of several steps: dissolution of precursor, some species rearrangement in liquid phase and finally polycondensation to the final product [3]. The structure of phosphate geopolymer is not resolved yet, there are at least four proposed structures and any of them is not fully proved and accepted [4]. However the influence of temperature on the properties is beyond doubt [5].

Phosphate geopolymers were prepared from metakaolin at several temperature from 25 to 80 °C. The reaction heat, evolved during the exotherm synthesis (measured by isothermal calorimetry), strongly increased with the temperature. The highest compressive strength was obtained in sample cured at 70 °C. The structural differences, caused by different kinetics of geopolymeration, were followed by ^{27}Al and ^{29}Si MAS NMR spectroscopy. This method proved more advanced reaction progress (from metakaolin to phosphate geopolymer) as result of higher curing temperature.

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Inorganic binders – as a way for sustainability iron casting productuon

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Keywords: sustainable development, clean casting production, new inorganic binders, volatile organic compounds emissions

The metal foundry industry in the European Union is a major employer, employing over 290,000 people. In addition, the importance of foundries to other industries is equally significant, as they provide a wide range of cast components for sectors such as automotive, shipbuilding, construction, defence and many others. For many years, in the technology of castings made in disposable sand molds, natural binders, resins and organic additives were used, which do not meet the currently applicable environmental requirements. For this reason, in line with the development of green technologies, efforts are being made to mitigate the negative impact of foundries on the environment, with particular attention to air quality [1]. This article presents research carried out within the new GREEN CASTING LIFE project (LIFE21 ENV/FI/101074439) [2], which is a continuation of the already completed GREEN FOUNDRY LIFE project (LIFE17 ENV/FI/000173) [3].The work carried out in the GREEN CASTING LIFE project will implement and validate at industrial level the use of inorganic binder systems for the production of molds in steel and iron foundries (achieving TRL8). This will have a very relevant environmental impact on the amount of harmful volatile and gaseous compounds emitted, on the indoor air quality for workers and on the waste generated by castings. The new knowledge gained will enrich the database needed to update the Best Available Techniques Reference Document for the foundry industry (SF BREF). The aim of the research is to demonstrate the potential benefits of using sustainable materials such as inorganic binders in European iron foundries in terms of improving the environment and working conditions through the introduction of cleaner and more ecological production methods and new innovative inorganic binders, and at the same time to provide a ranking of the binders tested in terms of their content of harmful substances. The article is the first to analyse seven novel, innovative inorganic binders and one organic binder (for comparison) in terms of the comprehensive emissions of gases from the BTEX group (benzene, toluene, ethylbenzene and xylenes) and PAHs (polycyclic aromatic hydrocarbons), as well as other compounds such as phenol, formaldehyde and isocyanates (MDI and TDI) and dusts (PM 2.5 and PM 10) generated during the process of pouring liquid metal into the mold [4, 5].

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High-temperature behaviour of ceramic high-entropy films from Cr–Hf–Mo–Ta–W–N system

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Keywords: high entropy nitrides, thin films, Cr–Hf–Mo–Ta–W–N, annealing, high temperatures

In general, high entropy alloys (HEAs) are multicomponent materials containing at least five principal elements. The research on HEAs was also extended to cover multicomponent ceramics, such as oxides, nitrides, carbides, and borides, due to their promising properties. High entropy ceramics can exhibit very good mechanical properties at low as well as at high temperatures, outstanding structural stability, and high oxidation resistance. This makes them promising candidates for next-generation replacements of traditional materials in many areas of the industry.

In the present study, we focused on the structure and properties of high entropy nitrides (HENs) from the Cr–Hf–Mo–Ta–W system. Cr–Hf–Mo–Ta–W–N films were prepared by magnetron sputtering at ambient temperature and at elevated temperature of 700°C. During deposition, the nitrogen flow was fixed to 20 sccm, while the target composition was changed in order to prepare thin films with a wide range of elemental compositions. The nitrogen content in the films was in the range of 35 – 52 at.%, and the content of metals in the films was changing in a wide range. After deposition elemental composition, structure and mechanical properties were investigated. Subsequently, the films were annealed in a vacuum to temperatures up to 1200°C and after cooling down to room temperature the structure and mechanical properties were examined.

It will be shown that appropriate deposition conditions result in the preparation of HEN films with a simple FCC structure given by the employed elements typical for high entropy nitrides with a hardness of 20 GPa. High hardness of these films is retained even after annealing to 1200°C in a vacuum. Changes in the structure after annealing will also be discussed.

T13: Kinetics and catalysis

Thermal behavior and kinetics of crude oil enhanced with copper nanoparticles: a thermogravimetric approach

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Keywords: thermogravimetry, combustion, nanoparticles, kinetic analysis

This study systematically examines the influence of copper nanoparticles on the thermal properties and reaction kinetics of crude oil through thermogravimetric analysis (TGA) under controlled laboratory conditions. Crude oil samples, each with a mass of 10 mg, were augmented with copper nanoparticles at concentrations of 10% and 20% by mass. The thermal decomposition was evaluated at five heating rates (5, 10, 15, 20, and 25°C/min) over a temperature range of 20–850°C in an atmospheric environment. Balance and sample purge gas flow rates were maintained at 80 ml/min (nitrogen) and 120 ml/min (dry air), respectively. The thermal decomposition exhibited two distinct reaction regions for all samples: (i) an initial region characterized by the evaporation of moisture, volatilization of light hydrocarbons, and fuel formation, and (ii) a primary combustion region marked by the oxidative degradation and burning of hydrocarbons. Copper nanoparticles significantly influenced the thermal behavior, with higher nanoparticle concentrations narrowing the reaction intervals and lowering peak combustion temperatures. Additionally, an increase in the heating rate caused a shift in peak temperatures to higher values and broadened the reaction zones. Kinetic analysis was conducted using model-free methodologies, including the Kissinger-Akahira-Sunose (KAS) and Ozawa-Flynn-Wall (OFW) methods[1], to calculate activation energies. The presence of copper nanoparticles reduced the activation energy, indicating their catalytic effect on crude oil combustion. These findings provide insights into the potential of copper nanoparticles to enhance the thermal performance of crude oil in industrial applications.

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Kinetic analysis of burnout of mineral-rich coal tailings for geopolymer applications

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Keywords: isoconversional method, kinetic parameters, deconvolution analysis

Leftover tailings from coal mining accumulate in slag heaps, causing significant environmental burden. However, these materials are often rich in kaolinite and other silicate minerals which are valuable in geopolymer preparation [1]. The main obstacle in such a valorization of coal tailings is the presence of organic and carbonaceous fraction. This non-mineral fraction can be removed via its complete transformation into gaseous products by oxidation at sufficiently high temperatures. On the other hand, excessive heating and long reaction times may lead to undesired transformation of certain amorphous phases into crystalline ones, which negatively impacts their suitability for geopolymer synthesis. Isoconversional kinetic analysis of thermogravimetric (TG) curves obtained in an oxidative atmosphere allows us to describe the burnout by means of kinetic parameters. Tailings from three different mining sites were analyzed, the burnout of non-mineral fraction was measured in dynamic air atmosphere at five heating rates in the 50–1000 °C temperature range. Figure 1 shows the typical TG and DTG curves obtained during heating; four distinct mass-change regions can be identified. Small initial mass loss (*i*) due to loss of weakly bound water below 150 °C is followed by transient mass gain (*ii*) probably caused by oxygen adsorption. The main oxidation stage (*iii*) proceeds in relatively narrow temperature range (400 °C to 600 °C); shift towards higher temperatures with increasing heating rate suggests kinetic control of the underlying oxidation processes. The final mass loss (*iv*) corresponds to dehydration and dehydroxylation of clay minerals. In this work, the mass loss during the main oxidation stage (*iii*) was isolated from the TG records in order to obtain the values of kinetic parameters unaffected by overlapping processes; deconvolution analysis based on empirical fitting functions [2] was employed.

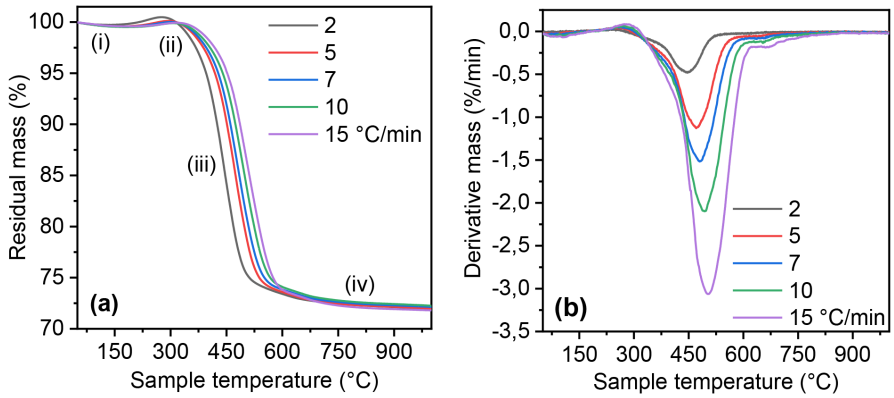

Fig. 1 Representative TG (a) and DTG (b) curves of coal mining tailings in air atmosphere

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Oxidation of soot by cerium dioxide synthesized under different hydrothermal conditions

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Keywords: cerium dioxide, hydrothermal conditions, particulate matter. thermogravimetric

In this study, a series of cerium dioxide catalysts with varying hydrothermal temperatures and times are synthesized by the hydrothermal method, without the use of templates. The impact of varying hydrothermal conditions on the activity of cerium dioxide catalysts is investigated through experiments to examin their oxidation characteristics in carbon fume combustion. Among the conditions tested, the hydrothermal conditions of 140 °C and 6 h yielded the most optimal catalytic oxidation of carbon smoke, with a combustion characteristic temperature (T_p) of 552 °C, and a reduction of 122.9 °C. The integrated combustion index (S) and combustion stability coefficient (R_w) are found to be 27.97×10^8 %²min-2 °C^{-3} and 90.76×10^5, respectively. The indices of S and R_w exhibit an improvement of 51.1% and 36.93%, respectively.

T14: Life sciences

Assessment of anti-cancer potential of harmaline: in vitro cytotoxicity and biocalorimetric analysis targeting nucleic acids

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Keywords: harmaline, beta carboline alkaloid, anti-cancer, Isothermal calorimetry ITC, binding affinity (K_b), binding stoichiometry (N), enthalpy change (ΔH_o)

Due to a lack of comprehensive knowledge regarding appropriate bio-target identification, specificity aspects, mode-mechanism of binding, and appropriate *in vitro* study, the use of small molecules as valuable drugs against diseases remains an indefinable purpose. Harmaline, an important beta-carboline alkaloid, exhibits potent anti-proliferative activity against several human cancer types and is also found to be a nucleic acid targeting natural molecule. Harmaline has been reported to show different signal pathways of apoptosis in different cancer cell lines and simultaneously characterize the structure activity aspects with different motifs of nucleic acid *viz*. CT DNA, poly A, poly(C).poly(G), and $tRNA^{phe}$, based on biocalorimetric analysis. The resulting data from ITC were analyzed to estimate the binding affinity (K_b), the binding stoichiometry (N) and the enthalpy change (ΔH^o). The free energy changes (ΔG^o) were calculated using the relationships, ΔG^o = -RT ln (K_b) and the heat capacity change ($\Delta C_p{}^o$) was obtained from the slope of the plots of variations of enthalpy with temperature.

The results open up new insights for the design and development of small molecule-based nucleic acid therapeutic agents.

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Retrieving pathway-specific substrate utilization rates from microbial heat flow curves

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Keywords: mycoplasma, monod equation, growth, metabolism, cell division

Isothermal microcalorimetry (IMC) is an extraordinarily sensitive tool for monitoring metabolic activities of microorganisms. It allows determining yields as well as rates of the underlying biochemical reactions. Although technically independent of each other, rates and yields may couple by metabolic regulation. Also experimentally, they are not always easily determined. The amount of metabolized substrate, required for yield estimates, is not always unambiguously obtained from time-integrated IMC curves ("enthalpy domain") and a multitude of growth models is used in a rather arbitrary way to model IMC data in the "time domain". These and other factors render comparability of IMC data from different labs difficult. Using the simplest glycolysis-based anaerobic metabolic network, i.e., that of the genome-minimized bacterium JCVIsyn3.b derived from the pathogenic group of Mycoplasma, we attempted a rigorous calorimetric analysis of metabolic yield and rate parameters. IMC data were modelled by an extended calorimetric Monod equation (ECME)[1] which applies to culture growth rather than substrate-dependent per-cell metabolic activity as originally defined by Monod. We identified pathway-specific heat yields for biomass- and non biomass-related metabolism and show how cell division rate an cell mass couple in response to the plasma membrane lipid composition in this smallest life-supporting system on earth. Using the validated benchmarks of heat flow modelling, we exemplify with IMC data from the fungus Schizophyllum commune – in transit from oxidative and fermentative metabolism –, how yield and rate estimates can be obtained systematically using the web-tool "Metabolator".

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Developing an energy-efficient responsibility model for the energy transition of shipyards

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Keywords: marine engine, bulk carrier, entropy, irreversibility, sustainability

The transition to renewable energy sources in shipyards is a pivotal step in the decarbonisation process, which entails a shift away from fossil fuels towards cleaner energy alternatives. This transition is characterised by a multifaceted approach, encompassing the adoption of energy-efficient technologies, implementing sustainable operational practices, and integrating renewable energy sources. It is of paramount importance to optimise energy consumption across major processes, including welding, material handling, and ventilation. Furthermore, alternative fuels such as hydrogen and biofuels must be investigated for their potential use in propulsion and auxiliary power. Furthermore, the transition requires investments in new infrastructure, retraining of the workforce, and potentially, collaboration between shipyards, suppliers, and regulatory bodies. The energy transition in shipyards is a complex undertaking with substantial economic and environmental implications, necessitating significant planning and investment to drive decarbonisation and ensure the long-term sustainability of the maritime industry and effective energy management. This study develops an energy management model for a real shipyard, leveraging the ISO 50001 standard to reduce energy costs and promote sustainability. The model, designed for a shipyard consuming approximately 1508 tonnes of oil equivalent (TOE) annually, identifies electricity (55%) and natural gas (45%) as primary targets for energy efficiency improvements. Key energy consumers, including welding machines, vehicles, cranes, air conditioning, and motor power units, are prioritized for targeted interventions. The model aims to create a sustainable energy management system, evaluating its overall cost-effectiveness and contribution to the shipyard's operational efficiency and environmental responsibility.

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T15: Materials science

Thermal-kinetic study of estonian clays and calcium/sulphur-rich industrial by-product under varied calcination atmospheres

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Keywords: thermal-kinetics-activation, clay, oil shale ash, flue gas

Non-kaolinitic clays, despite being abundant compared to kaolinitic clays, are underutilized as supplementary cementitious materials (SCMs) in concrete applications owing to their lower reactivity. Similarly, sulphur- and calcium-rich industrial by-products have been of limited utility compared to well-established SCMs like silica fume and ground granulated blast-furnace slag (GGBS), mainly because of their lower pozzolanic activity [1]. Estonia as a case study is relevant to this investigation, with large reserves of low-grade clays as well as a deposited reserve of landfilled oil shale ash (LOSA) amounting to hundreds of millions of tons [2]. Thermal activation provides a promising route to valorise these underutilized resources for applications such as in geopolymer, composite cements, and decarbonization schemes. To optimize thermal treatment, it is crucial to understand dehydroxylation and thermal decomposition mechanisms. Precise thermal characterization helps develop energy-saving activation parameters with minimal environmental impact, setting standards for industrial calcination and CO_2 capture integration. In this study, Estonian clays (Arumetsa-C, Kunda-C, Aseri-C) and LOSA were characterized by physical (Particle Size Distribution-PSD, Specific Surface Area-SSA) and chemical (X-ray Fluorescence-XRF, Fourier Transform Infrared Spectroscopy-FTIR, X-ray Diffraction-XRD) techniques. The effect of air and flue gas (16% CO_2 in N_2-O_2) on dehydroxylation kinetics for clays and carbonate decomposition for LOSA is investigated by simulating industrial calcination rotary kiln conditions. This investigation used a Setaram Setsys Evo 1750 thermoanalyzer with mass spectrometer (MS) and Advanced Kinetic and Technology Solutions (AKTS) software for kinetic analysis based on the model-free Friedman method (2.5-10 K/min heating rates). FTIR and XRD analysis provided complementary data on mineralogical transformations and phase evolution before and after thermal decomposition in both environments. The initial XRD analysis revealed that Arumetsa-C, Kunda-C, and Aseri-C contained kaolinite ranging from 2-16% and illite was the predominant mineral phase alongside smectite and mica. LOSA, consists primarily of calcite, comprising about half of the overall present phases. TGA-DTG-MS analysis showed that the clays had a major dehydroxylation peak (450-850°C) with H_2O evolution caused by removal of water from the illite, kaolinite, smectite phases, while LOSA displayed significant decarbonation (600-850°C) with CO_2 release owing to the presence of calcite. Most samples evolved a minuscule amount of SO_2 in both atmospheres. Switching from air

to flue gas slightly lowered peak dehydroxylation temperatures in the clays while raising LOSA's decarbonation temperature peak. The kinetic analysis revealed atmospheric effects across all samples, with flue gas hiking activation energy (Ea) for Arumetsa to ~200-250 kJ/mol from ~150 kJ/mol during the initial stages of the reaction (α=0.1-0.3), reducing Ea by 30-40% for Aseri and Kunda samples from ~200 kJ/mol to ~130-150 kJ/mol, then observed to raise Ea for LOSA to ~850 kJ/mol from ~270 kJ/mol at α=0.2. FTIR test revealed the absence of hydroxyl group (-OH) stretching vibration at 3600 cm^{-1} (dehydroxylation) and shifts on Si-O stretching was observed in all clays. LOSA sample showed a decreased carbonate (CO_3) absorption intensity (~1411 cm^{-1}) in air and then an intensity uptick in flue gas suggesting interaction with CO_2. The influence of flue gas on the dehydroxylation of clay minerals was negligible; however, the decomposition of carbonates exhibited greater sensitivity to variations in the partial pressure of CO_2.

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Pyrolysis of pvc and leather mixtures

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Keywords: TG/MS, Py-GC/MS, leather, PVC

Millions of tons of natural and synthetic leather wastes are generated every year in the automotive, fashion and other light industry sectors worldwide. Managing this complex waste is a challenging task [1]. Thermal treatment of the mixture could be a possible green solution of waste recycling instead of landfilling. The main advantage of this method is that separation of the waste components is not necessary. Polyvinyl chloride (PVC) and polyurethane (PU) are the two most common constituents of the artificial leather products. In this work, PVC powder mixed with natural leather in different ratios were chosen for modelling the synthetic and genuine leather waste material. It was found in our earlier study that the tanning agents had considerable impact on the quality and quantity of the decomposition products [2]. Therefore, variously tanned leathers, namely vegetable, chromium and mixed vegetable and aluminium tanned leathers were selected for this study. The thermal behaviour of the PVC-leather mixtures was studied in this work. The thermal decomposition pattern and the evolution profiles of some selected products of the mixtures and the pristine components were determined by thermogravimetry/mass spectrometry (TG/MS). It was found that in the presence of leather, the first decomposition step of PVC is shifted to a lower temperature range. Moreover, the amounts of the carbonaceous residues of the mixtures were lower than the values calculated from the TG curves of the pure components. For the detailed characterisation of the volatile decomposition products, pyrolysis-gas chromatography/mass spectrometry (Py-GC/MS) technique was used. Notable differences were observed from the expected composition of the pyrolyzate of the mixtures reflecting the interactions among the components during pyrolysis. Hydrogen chloride, a reactive gas evolves during the decomposition of PVC, which may interact with the decomposing leather resulting in a modified composition of the leather pyrolyzates. In order to prove this theory, co-pyrolysis of HCl solution and leather sample was studied by Py-GC/MS. The results showed that the hydrochloric acid is responsible for the increased hydrogen cyanide and methyl cyanide formation from the leather-PVC mixtures.

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Study of thermal behavior of adeka kiku-lube Z-112, a commercial ZDDP, and its tribology performance in lubricant etro 6

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Keywords: thermal degradation, phase transitions, lubricants, applied tribology, extreme pressure additives

Given our group's interest in the study of the thermal behavior of sulfur-based compounds [1] and the study of their tribology performance [2,3], herein, the thermal behavior and tribology performance of Z-112 as a commercial ZDDP additive, were investigated. Z-112, a commercial lubricant additive, was developed by ADEKA Corporation and exhibits high extreme pressure (EP) performance. It is a derivative of zinc di-alkyldithiophosphate (ZDDP) with a recommended dosage of 0.5-2.5% in lubricating oil. The thermal behavior of Z-112 was investigated at low to high temperatures using TG-DTA and DSC. Its degradation occurred through three steps with mass losses of 27.20, 28.65, and 16.95 wt. % at the range of temperatures of 285-330, 330-355, and 355-415 °C, respectively. Its degradation onset was at 311.09 °C, and an ash of 20.5 wt. % was detected at 600 °C. DSC revealed melting at −10 °C with ΔHfusion = −50.91 J/g and a crystallization point at −14.7 °C with ΔHfusion = 53.30 J/g. There is a broad exothermic phase transition without mass loss with enthalpy 190.14 J/g at the onset of 196.80 °C and endset of 269.03 °C. This phase transition was followed by stepwise degradation of Z-112. In addition, the tribology performance of Z-112 as additives in highly isoparaffinic Group III base oil, namely Petronas Etro 6, was evaluated using a four-ball friction and wear tester. Though the CoF of blend Z-112 was higher than Etro 6, the average wear scare area was smaller. The corrosivity of Z-112 as a commercial lubricant additive was observed due to its high sulfur content, however, its EP performance shows excellent results with high PB and PD values and a small wear scar area in high loading, supported by the FESEM-EDX.

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Use of thermal analysis to characterize composites obtained on the basis of diatomite, alumina or layered double hydroxides

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Keywords: uranium, adsorption, thermal decomposition, thermal analysis, diatomite, LDH, aluminium oxide

Natural layered silicates such as kaolinite and montmorillonite, which is the main component of mineral bentonite clays, have found wide application in industry, environmental technologies, food processing and pharmaceuticals. This is due to a combination of a number of physicochemical properties, such as high adsorption capacity, heat resistance, catalytic activity, high cation exchange capacity, and moisture retention capacity with low material cost and convenience of use. Diatomite, called diatomaceous earth, is also an interesting sorption material, and is a rock formed by the accumulation of diatom shells. It also contains iron compounds, clay minerals, quartz or calcite. An alternative to natural silicates is Double Layer Hydroxides (LDH), which also have a high specific surface area, high anion exchange capacity comparable to anion exchange resins and good thermal stability. LDHs are anionic materials comprising mixed layers of tetrahedral divalent metal hydroxide (M II (OH)) and octahedral trivalent metal hydroxide (MIII (OH)). These layers are held together by van der Waals forces (hydrogen bonds). Numerous biological and medical studies have shown that some LDHs (especially Zn Al, Ca Al, Mg Al) have very low toxicity and are in fact "friendly" substances. Moreover, due to their properties such as the ability to intercalate different types of anions (inorganic, organic, bio-molecules and even genes), high thermal stability, high biocompatibility and easy biodegradability, they can be materials with numerous biomedical applications. The aim of this research was to develop and test new multifunctional composite materials combining the properties of clays, diatomite, layered double hydroxides (LDHs). Such materials were tested for sorption properties and thermal stability. In view of their potential use in two very important fields: as sorbents for radioactive materials including radioactive wastewater containing uranium, and the second completely separate field is cosmetology, where these materials will act as sorbents AND carriers of active compounds such as anthocyanins, controlled-release vitamins. The thermal stability of the above composites was performed using STA 449 Jupiter F1 (Netzsch, Germany) equipped with a QMS 403D Aeo¨los mass spectrometer (Netzsch, Germany) and FTIR spectrometer (Bruker, Germany). NETZSCH ProteusÒ software, version 6.1. and the NIST library database were used. The purpose of the present study was to investigate the effect of the presence of adsorbates (e.g., uranyl ions, anthocyanins, chlorophyll) on the thermal stability of the tested sorbents. Unmodified LDHs are characterized by high thermal stability while the effect of the above adsorbates on their thermal stability is not reported in the literature. We used a thermogravimetric method combined with MS and gas-phase FTIR spectra to analyze sorption products,

such as U(VI), expecting to find an explanation for the mechanism of interaction of these ions with the adsorbent and their gradual decomposition with increasing temperature. On the basis of DTG curves of sorption products and gas-phase FTIR spectra of the decomposition of sorption products, it was determined that the thermal stability of silicate sorbents increased when U ions were sorbed, i.e. the temperature of defragmentation/oxidation increased. DSC curves of sorption products showed that defragmentation/oxidation was an exothermic process, while dehydration and dehydroxylation were endothermic. In the case of LDH, the differences in thermal decomposition temperature values were insignificant. For unmodified materials, three characteristic endothermic peaks were found in the DSC curves: the removal of physically adsorbed water, the mass loss corresponded to silicate dehydroxylation and thermal polymorphic transformation.

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Carbon dioxide emissions reduction through the development of ecological LC3 cement

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Keywords: CO_2 reduction, cement, clay, limestone, clinker

A significant advantage of LC3 cement, in comparison to conventional Portland cement (OPC), is its remarkable performance in terms of durability. The primary objective of this investigation is to synthesize LC3 cement utilizing diverse types of clay subjected to a water curing process lasting up to six months. The raw materials utilized encompass limestone, calcined clay, clinker, and gypsum. The calcined clays employed—montmorillonite clay and kaolinite—were subjected to firing at a temperature of 850 °C for duration of two hours, with a gradual heating rate of 5 °C/min. These clays were incorporated in varying proportions ranging from 30% to 45%, while limestone was added in quantities varying from 0% to 15%. The durability of the tap water was assessed over duration of six months. The performance assessment of the synthesized LC3 cement under aqueous curing conditions was executed utilizing a variety of analytical techniques, including X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), compressive strength evaluations, and scanning electron microscopy (SEM) for the specimens immersed in the solution. The findings indicate that the synthesized LC3 exhibits commendable durability in tap water for a period of six months, while the analysis of carbon dioxide emissions in comparison to conventional cement paste reveals a reduction in emissions of up to 50%.

High-entropy ($Ti_{0.4}Ta_{0.4}V_{0.4}Nb_{0.4}Cr_{0.4}$)AlC MAX phase synthesized by shs: structural, thermal, and mechanical insights

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Keywords: high entropy MAX phase, self-propagating high-temperature synthesis, oxidation resistance, spark plasma sintering

The concept of configurational entropy, or high-entropy (HE), has driven the development of a new class of materials – HE-MAX phases that possess exceptional structural and functional properties, making them promising candidates for applications in energy storage, catalysis, and thermoelectricity. Notably, their high-entropy structure can effectively reduce lattice thermal conductivity, which is essential for developing next-generation thermoelectric materials. However, the sustainable synthesis of HE-MAX phases has not been fully explored.

Self-propagating high-temperature synthesis (SHS) is an advantageous method which enables rapid, self-sustaining reactions, facilitating large-scale production with minimal energy input. SHS also ensures the formation of highly pure products with controlled microstructures due to its fast cooling and minimal contamination.

Here, we report the synthesis of equimolar 211 ($Ti_{0.4}Ta_{0.4}V_{0.4}Nb_{0.4}Cr_{0.4}$)AlC HE-MAX phase via energy-efficient SHS approach for the first time. The HE-MAX phase was designed by considering critical parameters such as crystal size, electronegativity, and valence electron concentration, ensuring the formation of a stable, substitutional single-phase material. It was observed, that high heating and cooling rates within the combustion wave promote favorable conditions for the formation of the 211 phase, demonstrating the potential of the SHS method for synthesizing this class of materials. DSC and TG analysis confirmed the enhanced thermal stability (up to 1200 °C) of the synthesized HE-MAX phase. The 211 HE-MAX phase exhibits superior oxidation stability compared to conventional MAX phases, maintaining structural integrity up to 620 °C. Furthermore, bulk samples were obtained from the HE-MAX powder using the spark plasma sintering (SPS) technique. These bulk samples exhibited significantly lower thermal conductivity (6.8 $Wm^{-1}K^{-1}$) and higher Vickers hardness (7.43 GPa) compared to conventional MAX phases, further demonstrating the impact of high-entropy stabilization on mechanical and thermal properties of material.

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Calo-IR: Development and first applications of an *in-situ* DSC-IR coupling

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Keywords: instrumentation, DSC, FT-IR, adsorption, Phase-Change Materials

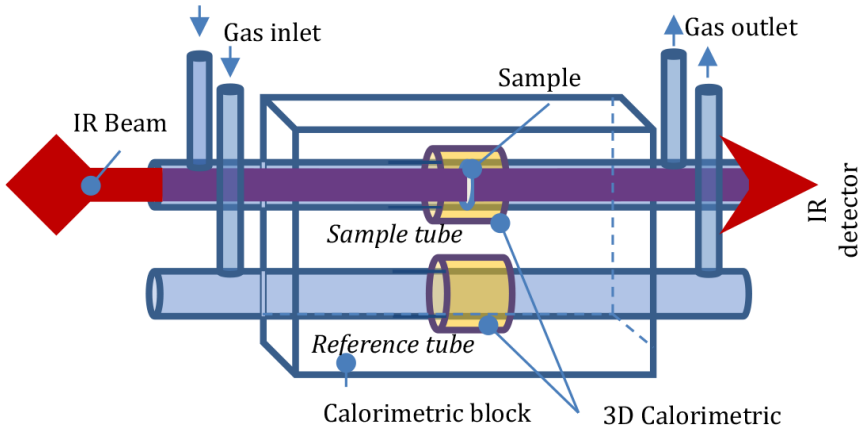
In this communication we describe the development, validation, and utilization of a device that couples *in-situ* infrared spectroscopy (IR) with differential scanning calorimetry (DSC). This setup directly links information about structural changes with the heat flow produced during transformations at the surface or within the bulk of the material.

The device combines a Tian Calvet micro-calorimeter (Setaram) with an FT-IR spectrometer (Thermo), further coupled to a mass spectrometer to analyze the gaseous flow exiting the sample compartment. In principle, this setup resembles a recently published DSC/Q-EXAFS coupling [1]. Major modifications included repositioning the calorimetric block within the spectrometer, adapting optical windows, and adjusting gas introduction systems to the calorimetric cell.

The device was validated through characterizing the surface properties of adsorbents and phase-change materials. The dual constraints of DSC and IR measurements necessitate minimal sample quantities; however, for the tested systems, this did not significantly affect the precision of IR and DSC measurements. Additionally, although the IR beam significantly impacted the thermogram baseline, it did not substantially affect the DSC signal.

By combining simultaneous information from both techniques, we provide a comprehensive view of a paraffin as a phase change material incorporated in an all cellulosic composite. We specifically determined simultaneously the structural/spectroscopic evolution of the materials undergoing a phase change while determining heat flows in repeated heating/cooling cycles, demonstrating the superiority of this coupling.

This unique setup ideally complements an in situ TGA-IR coupling (AGIR), previously developed in our laboratory [2]. Beyond the present application, the device's applications are broad, covering numerous areas in materials science. Its potential for elucidating and establishing more quantitative and reliable structure-property relationships will be discussed.



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Thermal and thermomechanical properties of laser-modified and electroplated thermoplastic polymer composites with electromagnetic field shielding properties

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The subject of this paper is to characterize the thermal and thermomechanical properties of laser-modified and electroplated thermoplastic polymer composites with electromagnetic field shielding properties. Suitable metallic fillers for the ABS polymer matrix and a laser modification technique were developed to enable selective electroplating of such composites. The conductive fillers used were copper (Cu) fibers and tin (Sn) powder in a total amount of 25 vol%, in varying proportions. The research focused in particular on the effect of these fillers on the thermal degradation processes of the developed polymer composites. The paper includes a detailed discussion and analysis of the test results: thermogravimetric Analysis (TGA), oxidation induction time and temperature (OIT), differential scanning calorimetry (DSC) and dynamic mechanical analysis (DMA). The main new functional features of the developed polymer composites (shielding properties and the possibility of selective electroplating) are also discussed.

Modeling of ultra-high-temperature complex borides synthesis using linear heating: effect of heating rate

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Keywords: ultra-high temperature materials, multicomponent borides, heating rate, reaction mechanism and kinetics

Complex Borides, a new generation of UHTCs, show promise with enhanced hardness and oxidation resistance compared to individual metal diborides. These materials find applications in aerospace, solar energy, metallurgy, and microelectronics. Ultra-High-Temperature Complex Borides (UHTCBs) exhibit a hexagonal lattice with mixed covalent and ionic bonds, combining advantages of high-entropy and ultra-high temperature materials. While promising, further research is needed to explore synthesis conditions, consolidation methodologies, and the intricate relationship between particle size, microstructure, and material properties for optimal applications. The synthesis of these advanced ceramics typically involves solid solution formation from commercial diboride powders using methods such as high-energy ball milling, borothermal reduction at 1,600 °C, molten salt synthesis at 1,100 °C, and borocarbothermal reduction at 1,850 °C under vacuum. However, these processes often introduce impurities, necessitating additional purification steps [1-2].

Addressing gaps, such as limited powder preparation methods, insufficient purity, high densification requirements, and potential grain growth during consolidation, not only advances UHTCBs but also unlocks tailored applications in nuclear fusion, solar power, and beyond, heralding a new era of material innovation and technological progress. One approach to addressing these gaps is modeling the process under controllable conditions, such as programmed heating and precise timing, using thermal analysis methods. By varying heating rates of reagents, it is possible to separate the stages and analyse intermediate quenched compounds for the exploration of interaction mechanism in the system under study. This research investigates the formation possibility and mechanism of (Hf,Nb,Ta,Ti,Mo)B_2 UHTCB material. This study utilized the high-speed temperature scanner (HSTS-3) device [3], enabling rapid and controlled processing of disc-shaped compressed Me+B mixtures at rates of up to 10,000 K/min and a maximum temperature of 2,000 K. Ex-situ characterization of materials linked reaction kinetics and phase transition mechanisms. Experiments with the multicomponent Hf-Nb-Ta-Ti-Mo-B system have shown that starting from a certain heating rate the interaction occurs through a single-stage exothermic reaction like thermal explosion by (Hf,Nb,Ta,Ti,Mo)B_2 formation**.** Moreover, as the heating rate increased, the exothermic stage shifted to higher temperature region. Experiments performed at various heating rates (100-2400 K/min) allow to determine the kinetic parameters (effective values of activation

energy) for the reaction using the Kissinger method. In addition, the heating rate plays a crucial role in the process's progression. Interestingly, with slower heating (100 K/min), no exothermic effect was observed on the heating curve. Nevertheless, the reaction proceeds, as evidenced by the presence of individual borides mixture in the cooled sample following the completion of heating.

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T16: Metals, alloys, intermetallics

Post processing thermal treatment of binder jetting 3D printed no-bake sand moulds

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Keywords: Binder Jetting 3D printing, furan no-bake moulds, sand moulds and cores, post processing thermal treatment, bending and tensile strength

The Fourth Industrial Revolution, currently underway, marks the next stage in humanity's pursuit of previously unimaginable advancements. Companies worldwide are striving to enhance the intelligence of their processes [1]. Only those that effectively utilise digitalisation, machine learning, and state-of-the-art production technologies will be able to maintain competitiveness in global markets [2].
The integration of additive manufacturing technologies in the foundry industry represents a revolutionary shift towards more efficient and optimised production processes. The application of additive manufacturing for sand moulds, among other benefits, enables the creation of complex geometries that were previously unattainable using conventional methods. A key advantage of this technology is the ability to produce sand moulds directly from CAD models, eliminating the need for costly core boxes or patterns [3]. This streamlined approach reduces project lead times and associated costs, significantly enhancing the efficiency of the entire production cycle [4].

Furan resin-based no-bake moulding technology has been employed in the industry for many years and has also proven to be highly compatible with additive manufacturing. However, a notable drawback of furan resin-based technology is the relatively slow setting kinetics of the moulding compound. To accelerate the curing process, the present study investigates the impact of post-processing techniques—heat and microwave treatment—on the strength of the moulding compound. In the case of 3D-printed sand moulds and cores manufactured using Binder Jetting technology, such treatments can significantly shorten the time required from mould production to its readiness for the pouring process, thereby improving overall process efficiency.

The specimens analysed in this study were manufactured using a KOCEL AJS 300A printer with Binder Jetting furan no-bake technology. After a curing period of two hours, the specimens were removed from the printer's work area, cleaned, and subjected to testing under three conditions: (a) without heat treatment, (b) after heat treatment, and (c) after microwave treatment. The heat-treated specimens were placed in an oven for 15 minutes at temperatures of 50°C, 100°C, 150°C, and 200°C. Microwave treatment was performed for two minutes at power levels ranging from 300W to 1000W.

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Application of the DTA method to analyze the crystallisation process of AlSi9Cu3(Fe) alloy with increased iron participation

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Keywords: the Al-Si-Cu cast alloys, DTA analysis, crystallization, iron content, scrap metal

The need to increase the proportion of scrap in feedstock is driven by the need to protect the environment by reducing the energy intensity of production and the amount of waste, reducing greenhouse gas emissions and the consumption of natural resources, and optimizing production costs. This also applies to metal products, of which aluminum and its alloys are the most recycled products among non-ferrous metals [1; 2]. Unfortunately, the increase in scrap content results in an increased proportion of many impurities, the worst of which, among metals, is iron. It crystallizes in the form of various phases, the most unfavorable of which is β-Al_5FeSi. Its lamellar-needle morphology with sharp edges and pointed corners results in the propagation of microcracks and stress concentration, which increases the brittleness of castings, hinders their machining, and reduces their mechanical properties [3; 4]. It is, therefore, essential to know the course of crystallization of Al-Si-Cu alloys with increased iron content and mainly to determine the sequence of phase transformations concerning the formation of β-Fe phases. The study includes cooling curves of EN AC-AlSi9Cu3(Fe)-EN AC-46000 alloy, into which iron (in the form of Al-Fe mortar - as a substitute for circulating scrap) was introduced with a content of 0.5 to 1.5wt.%. Crystallization analysis by thermal-derivative DTA and microstructure studies of the AlSi9Cu3(Fe) alloy with increasing iron content showed that up to about 0.4wt.%Fe, the iron phases formed do not significantly affect the crystallization and microstructure of the alloy. They are included in multiphase eutectics of the types α(Al)+(Al_2Cu,Fe)+β(Si) or α(Al)+($Al_XFe_YSi_Z$)+β(Si), which crystallize after the formation of the double eutectic α(Al)+β(Si). From about 0.5wt.%Fe to 0.9wt.%Fe, there is a pre-eutectic crystallization of iron phases, mainly the lamellar-eutectic β-Al_5FeSi At more than 1.0wt.%Fe, the morphology and size of this phase become even more unfavorable (due to primary crystallization) and is accompanied by numerous clusters of shrinkage porosity.

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The use of temperature analysis of DTA and DSC to crystallization of A390 alloy with melt overheating degree

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Keywords: the Al-Si cast alloys, DTA and DSC analysis, crystallization, melt overheating degree.

This paper presents the concept of superheating liquid A390 alloy (AlSi17Cu4Mg) to a temperature well above $T_{liq.}$, annealing it for a specified time, and casting it into a sand mold. A review of the literature [1;2] shows that such a process can be an alternative to the traditional method of modification of hypereutectic Al-Si alloys, causing fragmentation of primary silicon crystals β(Si) and their uniform distribution in the matrix of solid solution α(Al). The study was carried out for A390 alloy, which, due to its properties, mainly high strength and tribological resistance, is used in many industries, especially in the automotive industry, for castings of power trains (engine blocks and pistons). Based on previous own studies [3;4], it was found that the optimal superheating temperature is about 920-940°C, and the holding time is about 30 minutes. DTA thermal-derivative analysis and DSC scanning calorimetry were carried out for such conditions, recording the cooling curve and determining characteristic crystallization parameters. Direct determination of the parameters of high-temperature processes on a Multi HTC Setaram scanning calorimeter in an argon atmosphere allowed the determination of endo- and exothermic phase transformations and enthalpies of the components of the A390 alloy structure, i.e., solid solution dendrites α(Al), primary silicon crystals β(Si), double eutectic α(Al)+β(Si) and multi-component eutectics containing Al_2Cu and Mg_2Si phases. These parameters are needed to assess the thermal durability of engineering plastics, especially those with previously unconventional application areas, such as for heavily loaded castings operating under extreme thermo-mechanical stresses and tribological wear [5]. It was also found that overheating of the investigated alloy and the associated mode of heterogeneous nucleation caused significant fragmentation of β(Si) crystals to about 20-40μm with a morphology of compact lumps with a shape similar to octahedra.

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Dilatometric study of phase transformation kinetics In advanced 3mn bainitic steel subjected to isothermal heat treatment

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Keywords: bainitic steel, medium-Mn steel, retained austenite, phase transformation kinetics, dilatometry

One of the most promising materials for automotive forgings are medium-Mn bainitic steels which are part of the latest 3rd generation of Advanced High Strength Steels (AHSS). This type of steels contain 3-12 wt.% Mn. Their characteristic feature is the presence of retained austenite (RA) located between bainitic ferrite laths, which may transform into martensite during plastic deformation - TRansformation Induced Plasticity (TRIP) effect [1]. RA prevents the formation of microcracks by providing local plasticity, while the martensitic transformation of RA during plastic deformation contributes to blocking the propagation of possible microcracks. The combination of properly selected thermomechanical processing conditions and regulated cooling of forgings allows for obtaining a bainitic microstructure with fine lath-type RA, which is essential for obtaining high strength and improved cracking resistance [2,3].

In this work, the novel 0.17C-3Mn-1Si-0.5Al-0.2Mo-0.03Ti-0.07V type steel was investigated. The phase transformation kinetics during isothermal heat treatment was studied using dilatometric technique. The most optimal isothermal holding temperature (400°C) was selected for further dilatometric tests due to the highest amount of fine-lath type RA (10.3 vol.%) present in the microstructure after isothermal holding during 600 s. For this temperature variant, an influence of different isothermal holding times from 150 s to 1800 s was studied. In order to determine the amount of RA for particular time variants of isothermal holding step, X-ray diffraction (XRD) measurements were performed. In terms of the amount and stability of RA, the most optimal treatment variant was isothermal holding at 400°C for 900 s. A detailed microstructural analysis was performed using scanning electron microscope (SEM). The dilatometric results were correlated with hardness results. The research provides the basis for the further optimization of the processing parameters of investigated steel.

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T17: Nanofluids

Numerical investigation of chemical reactive mhd fluid dynamics over a porous surface with cattaneo–christov heat flux

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Keywords: Arrhenius energy, Williamson fluid model, 3D flow, Cattaneo–Christov heat flux, Levenberg–Marquardt approach

A theoretical framework to investigate three-dimensional Williamson fluid flow over a bi-directional extended flat horizontal surface is proposed in this dissertation. Artificial intelligence and machine learning fields have seen tremendous prominence along with the rapid advancement of related technology. This work trains a machine learning model based on artificial neural networks to handle the mathematical formulation incorporating heat source and Hall effects using the Levenberg–Marquardt approach (LMA). Additionally, the impact of activation energy on fluid concentration is incorporated into the analysis. Cattaneo-Christov double diffusion models are used to model heat transfer combined with the effects of thermal radiation. The solutions, serving as reference datasets for various scenarios, have been generated numerically using the BVP4C approach. Artificial neural networks are utilized for training, testing, and validating these numerical computations using a 70:15:15 ratio. The predictive model accuracy is evaluated using various statistical metrics, including linear regression, histograms, fitting analysis, and mean squared error evaluations, with the least error ranging between 10^{-3} and 10^{-4}, based on individual error analysis of four parameters. The findings show that temperature rises with the *M* parameter, whereas velocity declines by increasing the *M* parameter. Concentration rises with increasing activation energy parameter and falls with decreasing *Sc*. The results show that artificial neural networks can provide a successful replacement for forecasts for the future, and the fluid flow structure simulated here may result in better industrial designs.

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Stability and thermal conductivity of carbon nanotube – oxide type hybrid nanofluids

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Keywords: nanofluid, carbon-nanotube, titanium-dioxide, silicon-dioxide, thermal conductivity, viscosity, stability

Nowadays our modern society needs more energy than ever before. Efficient energy utilization is a hot topic that is quite popular amongst researchers. One way to do so is to increase the efficiency of heat exchangers that are all around us in our everyday lives. Heat exchange depends on several factors like temperature difference, contact area and the thermal conductivity of involved matter. Heat exchange can be improved by modifying the thermal conductivity of the working fluid and by this the efficiency of the heat exchanger can be improved or the size of it reduced. Choi and Eastman are the forerunners of nanofluids, which are engineered dispersions containing high thermal conductivity nanoparticles and conventional working fluids as the continuous phase. [1,2]

We prepared multi walled carbon nanotube (MWCNT) and hybrid nanofluids with the addition of silicon- or titanium-dioxide in a volume ratio of 1:1 with the MWCNT in multiple concentrations. We characterised the rheological and thermal behaviour of the nanofluids and examined their stability through zeta potential and aggregate size analysis. We achived a maximal increase in thermal conductivity with 5000 ppm(vol/vol) MWCNT nanofluid at 5.7% (20 °C). We found that the MWCNT content has the primary effect on thermal conductivity, but in terms of stability, the aggregate size is smaller with the addition of oxide nanoparticles. We propose that during the ultrasound treatment the oxide particles promote the disentanglement of the MWCNTs. It is promising to further study this effect on different concentrations. In these hybrid nanofluids the carbonous part could be responsible for the enhanced thermal properties, while the added oxide contributes to the building up and maintaining of stability.

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Optimizing thermal performance of heat sinks using ZnO-integrated phase change materials for sustainable energy solutions

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Keywords: unfinned, copper foam, ZnO nanocomposites, RT-54HC (PCM), clean energy storage solution, zero emission thermal management

Electronic devices generate significant heat during prolonged operation, making efficient thermal management crucial to maintain performance and prevent premature failure. Traditional phase change materials (PCMs) have been widely used for passive cooling due to their ability to absorb and release heat during phase transitions. However, their inherently low thermal conductivity limits their efficiency in high-performance, temperature-sensitive systems. To address this challenge, the present research explores the integration of zinc oxide (ZnO) nanocarriers into RT54HC PCMs to develop nanocarrier-based phase change materials (NcPCMs). The goal is to enhance the thermal conductivity and overall cooling capacity of heat sinks. The thermal behavior of ZnO/RT54HC NcPCMs was investigated across transient heat loads and varying ZnO saturation levels.

The results demonstrated that both simple and copper foam-embedded heat sinks achieved notable temperature reductions when ZnO nanocarriers were incorporated into the cooling media. Compared to unfilled, unfinned heat sinks, the NcPCM-based copper heat sinks significantly reduced peak temperatures and extended operational times at different critical temperatures.

These findings highlight the potential of nanocarrier-enhanced PCMs in advancing sustainable thermal management solutions. By leveraging environmentally friendly, zero-emission cooling technologies, this research promotes clean energy storage and supports the development of more efficient electronic systems. The study advocates for further integration of nanotechnology and thermal engineering to address the growing demands of modern electronic devices.

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Impact of activation energy and motile microorganisms on casson nanofluid flow across an exponentially curved surface

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Keywords: curved surface, casson fluid, MHD, microorganism, activation energy, bio-convection

This research provides a detailed analysis of the two-dimensional magnetohydrodynamic (MHD) flow of a Casson fluid across an exponentially stretching curved surface, considering the presence of motile microorganisms. The study integrates Darcy flow, variable thermal conductivity, and activation energy effects. It investigates the momentum and energy characteristics of the Casson fluid under Darcy flow conditions, while also assessing the role of activation energy in shaping the concentration profile and analysing bioconvection dynamics in the microorganism distribution. A thorough parametric analysis is performed to evaluate the influence of critical factors such as the Casson fluid parameter, permeability, Brinkman number, activation energy, and bio-Schmidt number on velocity, temperature, concentration, and microorganism profiles. The governing partial differential equations (PDEs) are converted into ordinary differential equations (ODEs) using similarity transformations. The resulting boundary value problem is numerically solved using the BVP4c technique in MATLAB. The findings emphasize the effects of various physical parameters on the Sherwood number, Nusselt number, skin friction coefficient, and local motile microorganism density, offering significant insights into the intricate interactions of fluid dynamics, heat transfer, and mass transfer in systems involving bioconvection and chemical reactions. This study advances the understanding of non-Newtonian fluid behaviour in porous media, with potential applications in engineering and biological processes.

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Enhancement of the performance of a spherical distiller using hybrid nanofluids

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Keywords: water desalination, solar distillers, hybrid nanofluids, thermal properties, environmental impact

Solar distillers represent a practical way for water desalination using solar energy. Water scarcity appears to be a challenging problem to be solved using different techniques. In this research, the performance of solar distiller was investigated using hybrid nanofluids. The hybrid nanofluids, combined two or more types of nanoparticles suspended in a base fluid, offered superior thermal properties to traditional nanofluids. The research investigated the impact of various hybrid nanofluids on the efficiency of the distillation process, focusing on heat transfer rates, evaporation rates, and overall water production efficiency. Experimental measurements were conducted using different combinations of different percentage in the range of 0.25 to 2.5 wt./v % nanoparticles. The nano materials used were Al_2O_3, carbon nanotubes, and graphene nanotubes. The results demonstrated that using hybrid nanofluids significantly improved the distiller's productivity. The optimal combination of nanoparticles for maximum performance enhancement were identified. Furthermore, a comprehensive analysis of the economic viability and environmental impact of using hybrid nanofluids in spherical distillers was performed. The findings of this research offered valuable insights for the design and optimization of advanced distillation systems, highlighting the potential of hybrid nanofluids to revolutionize the field of thermal desalination.

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PEG based nanocolloids for heat transfer applications: a study on heat transfer enhancement in laminar flow

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Keywords: nanocolloids, PEG 400, heat transfer coefficient, laminar flow

Nanocolloids for heat transfer applications are not a new area; however, there is intense research on different nanoparticles and base fluid combinations in order to find the best option for a specific application. This article is based on a coordinated experimental study on PEG 400 with three kinds of nanoparticles: two oxides (MgO and alumina) and multi wall carbon nanotubes (MWCNT). A polyethylene glycol (i.e. PEG 400) was considered as base fluid and the prepared nano suspensions were analysed in terms of thermophysical properties, as are detailed in [1-7]. The nanoparticle concentrations were as follows: 0.5 – 2.5 %wt. for Al2O3 and ZnO and 0.025 – 0.1 %wt, for MWCNT, resulting in a number of 12 fluids that were experimental investigated (see [2-4, 6, 7] and further compared numerical in terms of laminar heat transfer performance. The numerical model was carefully validated and the mesh was calculated in order to give trustable results. The geometrical configuration of the model was a 2D tube with two zones: an isothermal zone at 293.15 K and a heating zone of 8000 W/m^2. The numerical analysis was performed employing Ansys workbench 17 for different Reynolds number in laminar flow (i.e. Re = 500 – 2000). Results were collected in terms of exit temperatures (medium and maximum temperature at tube exit) and Nusselt number, followed by heat transfer coefficient calculus. The numerical results revealed that Nusselt number increases with both Re number, which is a logical phenomenon, and with the nanoparticle addition, confirming the theory that the nanofluids performance in laminar flow is superior of that of the base fluid. More exactly, at Re = 500, for PEG 400 + Al2O3 nanocolloid, the increase in heat transfer coefficient is up to 6.4 %, while for ZnO and MWCNT the augmentation is up to 13.02 and 13.83 %, respectively. Another observation is that the heat transfer enhancement decreases with the increase in Re number and this phenomenon appears due to the high viscosity of the suspensions. Concluding, the PEG 400 nanocolloids with both oxides and MWCNTs perform well in laminar heat transfer and can be an option for medium heat exchange applications, especially due to the large thermal stability of PEG 400 (see [4] for details on thermal stability).

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Preparation and investigation of hybrid and composite SiO_2-Zno nanofluids

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Keywords: nanofluid, SiO_2, ZnO, dispersion, rheology, thermal conductivity

Nanofluids are phase colloids in which nanoparticles are dispersed in a liquid to obtain a dispersion with enhanced thermal properties – such as increased conductivity or higher heat capacity – compared to the base fluid. It has long been known that solid materials have higher thermal conductivity than liquids. However, Choi and Eastman were the first to disperse small enough solid particles into a liquid with the goal of increasing thermal conductivity at the end of the last century [1].

Enhancing heat transfer using nanofluids with improved thermal conductivity is particularly beneficial when traditional options, such as increasing the heat transfer area or using larger temperature difference, are not practical. While the concept may seem simple, nanofluids present several challenges that require extensive research. Nothing illustrates this better than the exponential increase in published articles on the subject over the past three decades.

To predict the properties of complete nanofluids, it is important to understand both the nanoparticles and the base fluid. While traditional base fluids are well known, nanoparticles require further research – especially regarding the behaviour of the different suspended particles in the dispersions. For nanofluids to be economically viable, they must be safe, effective and cost-efficient. A safe nanofluid not only non-toxic, incombustible, non-explosive, but also the particle aggregation is also inhibited into larger clusters that could clog the equipment in which it is used. Effectiveness is a straightforward criterion: the particles should significantly enhance thermal conductivity without causing a decent increase of viscosity. Additionally, nanofluids are more expensive than base fluids, meaning they will only be used if their benefits outweigh their production costs. More and more companies are selling industrially made nanoparticles nowadays. Due to economies of scale, these are much cheaper than particles produced in laboratory batches. However, while the availability of these particles is great, it has not led to a major breakthrough in the nanofluid application. This is because, during drying and storage the particles tend to aggregate (drawbacks of two steps method).

In my research hybrid and composite SiO_2-ZnO nanofluids were synthesized and analysed. The nanoparticles and nanofluids were prepared using various methods, including sol-gel, atomic layer deposition, and both one-step and two-steps methods. The nanoparticles, their aggregates in the dispersion and the nanofluids were examined using a range of analytical and material science techniques such as electron microscopy, infrared and optical emission spectroscopies, dynamic light scattering, viscometry and thermal conductivity measurements (modified transient plane source)

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T18: Nanomaterials and composites

Influence and accuracy of micro vs macro scale thermal characterization in wall-board PCM-gypsum composites

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Keywords: thermal characterization, thermoregulating gypsum composites, differential scanning calorimetry, heat capacity, thermogravimetric analysis, composite characteristics

Incorporating phase change materials (PCMs) into building components can endow them with thermoregulating properties, allowing to store waste heat within narrow temperature ranges and thereby reducing temperature fluctuations to enhance indoor thermal comfort. Previously, we have reported not only the manufacturing of liquid Nanosized Phase Change Slurries (NPCSs) [1,2], but also their successful application for preparing gypsum composites with thermoregulating properties containing nanoencapsulated PCMs[3]. Although the overall thermal storage capability of these gypsum composites has been proved [3] certain properties remain unclear. For instance, a non-uniform dispersion of nanocapsules within the gypsum matrix can make more complex the characterization process, as it may lead to a heterogeneous distribution of thermal properties (conductivity, heat capacity, or even latent heat storage). Consequently, the sampling process plays a critical role in determining small-scale thermal characterization techniques such as thermogravimetry (TGA) or differential scanning calorimetry (DSC). To mitigate these problems, alternative macro-scale characterization techniques need to be developed to estimate the thermal properties of the entire composite. So, in this work we have carried out a characterization technique to assess with precision the latent heat thermal storage of gypsum composite blocks containing encapsulated PCM with big area (30 cm x 30 cm) employing a Heat Flow Meter (HFM) originally conceived for conductivity measurements. The heat capacity of the samples was measured as a function of temperature, enabling the separation of sensible and latent heat contributions, and thereby allowing the determination of the composites' overall latent heat storage capacity. The results reveal that the latent heat of the gypsum block composite was independent of the dynamic conditions applied during measurement, in contrast to microscale measurements, where results typically depend on the heating rate. Moreover, while sampling for DSC measurements results critical, as variations arose from the heterogeneity of the gypsum sample, this approach enables assessment of the entire gypsum block composite simultaneously, thereby avoiding sampling errors or variations. We consider the characterization method here presented can pave a route toward a proper measurement protocol for thermoregulating building materials.

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Modified zinc-oxide based photocatalysts on clay mineral surfaces

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Keywords: photocatalyst, thermogravimetry, kaolinite, halloysite

Conventional water treatment technologies are often not effective enough to remove organic components such as pesticides and pharmaceutical residues. This is when alternative solutions, which although smaller in capacity and often more expensive, can be more effective. One option is the use of heterogeneous photocatalysis, where the photocatalytic nature of metal-oxides (e.g. TiO_2, ZnO) can be exploited to degrade organic contaminants. The efficiency of single component oxides can be increased by using mixed oxides, where a composite system of two or more metal oxides is formed. This can improve surface properties (e.g. specific surface area, pore structure), reduce photocorrosion and aggregation, and increase photon utilization, thus shifting the operating range from the UV to the visible range.

The photocatalytic property of ZnO has been known for a long time, and its efficiency is approximate to that of TiO_2, which has already been widely used [1]. However, it requires higher energy UV photons for excitation and is also prone to photocorrosion. Combination with Cu or Ni oxide is aimed at overcoming these disadvantages [2]. It is assumed that similar effect can be achieved with a composite containing In-oxide [3]. A proper surface structure of oxide composites can be achieved if the oxides are not only physical mixtures, but their formation occurs in parallel from the precursor salts given during the heat treatment preparation.

In this work, Cu- and In-modified ZnO mixed oxide composites and their deposition onto clay mineral surface were studied. The applied clay minerals (kaolinite, halloysite) act as catalyst supports to prevent the aggregation of oxides, in addition, have moderate but detectable intrinsic photocatalytic nature [4, 5].

Metal oxides were prepared from precursor salts by precipitation and thermal treatment. In order to determine the composition with the most effective photocatalytic character, samples with different oxide-to-mineral ratios were prepared. Two different clay minerals were used as catalyst support, differing in hydration, morphology and photocatalytic activity. The phase composition of the samples was verified by XRD and the surface molecular structure was studied by FTIR-ATR spectroscopy. Thermogravimetry (TGA) was used to monitor the thermal decomposition processes. TGA results were also used to determine the treatment temperature. The photocatalytic activity was investigated in aqueous medium with coumarin, a ·OH radical scavenger test compound. The concentration of 7-hydroxycoumarin produced from coumarin was measured by fluorimetry. Since the photocatalytic activity is strongly dependent porosity, N_2 adsorption experiments were carried out to determine specific surface area and pore size.

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T21: Polymers

Study of semi-crystalline copolymers by differential scanning calorimetry

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Keywords: copolymers, crystallinity, DSC

Block copolymers are increasingly used in industrial applications due to the diverse and complementary properties of each block. The synthesis routes give the opportunity to control the length and ratio of each block, providing the copolymer with highly specific properties. Because of their many physicochemical characteristics, block copolymers are finding use in a wider range of fields, from biology or medicine to chemistry, physics, and materials science. With a hydrophilic polyethylene glycol (PEG) block and a hydrophobic polyethylene (PE) block, polyethylene-block-polyethylene glycol copolymers (PE-b-PEG) are amphiphilic di-block copolymers. Furthermore, both blocks are able to crystallize, in two different crystalline phases. This study aims to investigate the crystallinity of PE-b-PEG copolymers with varying ratios of PE and PEG blocks and examine how the composition of the copolymers affects their crystallization. The characterization of different PE-b-PEG copolymers with varying compositions will demonstrate the effects of the molecular weight and the weight ratio of the two polymer blocks on the PE-b-PEG crystallinity. Differential Scanning Calorimetry (DSC) will be used to study the endothermic melting peaks and exothermic crystallization peaks of copolymers and to determine the crystallinity degree of each block, through the melting enthalpy. The copolymers' PE/PEG block ratio ranges from 17/83 to 77/23 (weight/weight). The experimental results demonstrated that the crystallization of one block is favoured when the ratio of that block is increased. One very broad large endothermic peak attributable to the melting of the PE crystalline phase is indeed seen for a PE-b-PEG copolymer containing 77% PE, and no crystallization of PEG block is observed. A DSC analysis of a PE-b-PEG copolymer, which is composed primarily of PEG blocks, was also conducted to determine how the blocks ratio affects the copolymers' thermal characteristics and crystallinity. For copolymer contains 83 % of PEG, the DSC thermogram are very similar to the one seen for the PEG homopolymer, on no PE crystallization is detected. For a composition close to 50/50, DSC results have shown that both blocks can crystallize. Consequently, an increase in the ratio of one block promotes the crystallization of that block while impeding or even preventing the crystallization of the other block [1]. DSC appears to be a fruitful technique to investigate the crystallinity of PE-b-PEG diblock copolymers which can have a significant influence on the organization of such copolymers when they are adsorbed on a solid substrate or at a liquid interface for surfactant or lubricant applications [2].

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Thermal behaviors and crystallization properties of new silicone-based polymers

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Keywords: silicones, copolymers, DSC, thermal properties

A wide range of attractive properties, including a low glass transition temperature (-120 °C), high chain flexibility, high resistance to chemical oxidation, high thermal and UV stability, marked hydrophobic character, and high biocompatibility, make silicone polymers very interesting polymers for industrial applications. Because of their low solubility parameter, they exhibit thermodynamic incompatibility with the majority of other polymers and have relatively poor mechanical properties despite their unique characteristics. Moreover, because silicone polymers have a strong tendency to dewet when deposited on solid surfaces, they have limited applications as coating for controlling chemical surface modification. Synthesis of original block copolymers with a viscoelastic polydimethylsiloxane (PDMS) block were realized, and their thermal properties studied [1] in order to improve their chemical compatibility and applications as coatings. PDMS was copolymerized with caprolactone (CL) and lactic acid (LA) which are currently being reconsidered with particular attention because of their good biodegradability. Thus, by combining the surface-modifying and toughening properties of PDMS with the compatibilizing properties of polycaprolactone (PCL) and polylactic acid (PLA), block copolymers based on PDMS and PCL or PLA are relevant solutions for applications as biomaterials, drug encapsulation, and surface-modifying additives.

PDMS-block-PCL (diblock, triblock, and star) and PDMS-block-PLA (diblock and triblock) copolymers were synthesized by ring-opening polymerization of CL and LA, respectively, with hydroxyl-terminated PDMS oligomers serving as initiators. FTIR, SEC, and ^{1}H NMR spectroscopy experiments confirm the formation of the desired structures. Thermal transitions (glass transition, crystallization and melting temperatures), corresponding enthalpies and degrees of crystallinity of the various copolymers where investigated using differential scanning calorimetry (DSC). Thermal analyses were performed with a TA Instruments Q200 differential scanning calorimeter. For block copolymers containing a PCL block, thermograms were recorded between -90°C and 150°C with a heating rate of 10°C.min^{-1}. For block copolymers containing a PLA block, thermograms were recorded between -90°C and 20 °C with a heating rate of 10°C.min^{-1}.

The findings, for PDMS-block-PCL copolymers, show how intricately polymer structure and PCL block length affect the PDMS block's crystallization. The crystallization of PCL blocks, in diblock copolymers, was caused by the stacking of adjacent chains, which caused the PDMS block to extend and crystallize more readily. Because both PCL end-blocks participate in the same PCL lamella, folding of PDMS chains may be significant in triblocks. As the length of PCL blocks increases, a limited crystallization of PDMS is seen in star copolymers, exhibiting the same tendency as in triblock copolymers. Melting and crystallization transitions of PLA blocks are never seen in PDMS-block-PLA copolymers. Consider-

ing diblock copolymers, PDMS sequences can crystallize, and for PLA block the degree of crystallinity stays high and rather constant for PLA block molecular weight between 900 and 9900 $g.mol^{-1}$. Higher PLA block molecular weight causes a sharp decrease in crystallinity. The increase of entanglements between copolymer chains for high molecular weight, which inhibits further crystallization, is most likely the cause. Finally, because the PDMS block is sandwiched between two amorphous PLA blocks, it cannot crystallize in PLA-block-PDMS-block-PLA tri-block copolymers.

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Relationship between structure and thermal properties of sustainable polyurethanes synthesized with the use of bio-based diisocyanates

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Keywords: thermal properties, chemical structure, bio-based diisocyanates, polyurethanes, sustainable production

Nowadays in the synthesis of polyurethane materials (PUs), sustainable components play a crucial role. Incorporating bio-based monomers into their chemical structure is one of the most promising strategies for developing greener production methods of this kind of polymers. Typically, bio-based polyols and glycols are used as key raw origin components. In this work, we propose the use of bio-based diisocyanates synthesized via the Curtius rearrangement for PU synthesis.

The aim of this study is to investigate the relationship between structure and thermal properties in sustainable polyurethanes synthesized using bio-based diisocyanates derived from biologically sourced dicarboxylic acids. In the first step of the PU synthesis process, two types of bio-based diisocyanates (BIO-ISO) were obtained via the Curtius rearrangement. Succinic and azelaic acids were used as precursors, which were initially converted into diacid chlorides through reaction with thionyl chloride, followed by transformation into the corresponding acyl azides using sodium azide. Upon thermal treatment, each acyl azide was converted into the respective bio-based diisocyanate. The structure of the obtained diisocyanates was confirmed using Nuclear Magnetic Resonance (^{1}H NMR, ^{13}C NMR) and Fourier Transform Infrared Spectroscopy (FTIR).

The synthesized diisocyanate compounds were used to produce sustainable polyurethane (PU) materials via the prepolymer method. In the first step, a urethane prepolymer was synthesized through the reaction of BIO-ISO with polyester polyols. In the second step, the prepolymer underwent chain extension using bioglycols (1,4-butanediol and 1,3-propanediol) in the presence of dibutyltin dilaurate as a catalyst. All PU samples were prepared with a final molar ratio of isocyanate to hydroxyl group equalled 1.0. The resulting PU materials were analysed using FTIR spectroscopy and thermally characterized by Differential Scanning Calorimetry (DSC) and Thermogravimetric Analysis (TGA).

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Thermoanalytical approach to assess riverine pet litter and its recycling potential

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Keywords: riverine litter, circular economy, PET bottles, thermal analysis, environmental ageing, mechanical recycling

Due to inadequate waste management and extreme weather phenomena, a concerning amount of plastic waste enters the rivers and gets transported into oceans and seas, where their collection is challenging. Apart from the fact that macroplastics disturb the aqueous ecosystem, microplastics – generated by the degradation of larger particles – might pose a greater risk as limited information is available on their effect on living organisms[1]. Therefore, it is vital to catch the plastic floods while they are in the rivers and collect information on their properties to find the most suitable waste management/recycling option for these plastic streams.

For this purpose, we developed a thermoanalytical method based on differential scanning calorimetry (DSC) to quantitatively link the crystallization dynamics of bottle-grade poly(ethylene-terephthalate) (PET) with its degradation state[2]. The study uniquely simulated long-term sunlight exposure through controlled artificial ageing of PET bottles in a Xenon chamber, with degradation levels accurately determined via intrinsic viscosity (IV) measurements. Following degradation, DSC analysis was conducted, and the complex melting endotherms observed during the post-isothermal crystallization heating phase were deconvoluted into sub-peaks using the Fraser-Suzuki function.

A progressive discovery was made: a specific sub-peak exhibited a melting temperature with a strong, linear relationship to the molecular chain length of PET, providing a precise indicator of polymer degradation. This correlation represented a significant advancement in the field, as it was successfully applied to PET litter samples collected from floodplains in Hungary within the catchment area of the Tisza River, enabling accurate estimation of environmental degradation levels. Moreover, based on the determined IV ranges of the riverine PET bottles, we proposed targeted recycling strategies for this pervasive pollutant, with a comprehensive evaluation of reprocessing outcomes.

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Green epoxy vitrimers enhanced with liquid crystalline phase

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Keywords: epoxy resin, self-healing, DSC, POM, liquid crystals, polymer network

Epoxy vitrimers are a promising class of materials that combine the superior mechanical properties of thermosets with the recyclability and self-healing capabilities. However, their widespread application is hindered by the necessity of toxic catalysts that facilitate bond exchange reactions. In this study, we present a novel, catalyst-free epoxy vitrimer system modified with a liquid crystalline epoxy resin (LCER) to enhance its dynamic properties while maintaining a sustainable, green chemistry approach.

To achieve this, an LCER was specifically synthesized and incorporated at 10 wt% into a base epoxy system composed of a diglycidyl ether of bisphenol A (DGEBA) resin and an anhydride hardener. Two anhydrides, maleic anhydride (MA) and phthalic anhydride (PA), were evaluated as curing agents to determine their impact on the vitrimeric and mechanical properties of the resulting networks. The study revealed that the systems cured with an aliphatic anhydride exhibited superior and self-healing characteristics compared to their aromatic counterparts. Moreover, the use of MA allowed to use lower curing temperature and achieve uniform samples.

A critical innovation in this work was the replacement of conventional toxic transesterification catalysts, such as zinc or tin compounds, with an excess of glycerol and addition of the LCER as a green alternative. Glycerol, a biodegradable and non-toxic polyol, facilitated dynamic covalent bond exchange, thereby enabling stress relaxation and self-healing without compromising the structural integrity of the material.

Differential scanning calorimetry (DSC) was employed to analyze the thermal behavior of the resin and its compatibility with the epoxy vitrimer network as well as curing process itself and thermal characteristics of the obtained polymer network. Hot-stage polarized optical microscopy (hs-POM) was used to confirm the formation of liquid crystalline phases of the LCER and to track the healing process.

Furthermore, it was observed that in selected formulations, the addition of LCER itself was sufficient to induce self-healing capabilities without the necessity of any multi-hydroxyl alcohol. The unique liquid crystalline domains within the epoxy matrix acted as self-repairing units, enabling damage recovery under thermal stimuli. The developed system provides a sustainable alternative to traditional epoxy vitrimers by eliminating hazardous catalysts while maintaining recyclability performance thus extending the materials lifespan. The dual functionality of the LCER, acting both as a structural enhancer and a self-healing promoter, represents a significant advancement in the field of green polymeric materials.

Future studies will focus on optimizing the composition and processing conditions to further improve the efficiency and applicability of these catalyst-free epoxy vitrimers in advanced engineering applications and on more detailed characterization of the properties of the networks.

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Application of a natural antioxidant, gallic acid, as a stabilizer in polyethylene

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Keywords: natural antioxidant, gallic acid, polyethylene, stabilizer, degradation

Polyethylene (PE) products usually contain a hindered phenolic antioxidant as the primary stabilizer and a phosphorus or sulfur-containing compound as a secondary stabilizer to hinder their degradation during processing and application. Recently, however, the interest in natural, bio-based products has increased considerably in all areas of life, including stabilization. Some time ago, concerns were expressed about the possible harmful effects of the hindered phenolic antioxidants widely used in products in contact with water or food [1]. Nature produces and uses numerous compounds with strong antioxidant effects, including lignin, flavonoids or flavonols, curcumin, and many other polyphenolic compounds, like gallic acid.

Gallic acid (GA) was characterized with different thermoanalytical methods (DSC, TGA). Polyethylene was mixed with GA and extruded multiple times in the presence and absence of PEPQ, a secondary phosphorus antioxidant. As a reference, an industrial phenolic antioxidant, Irganox 1010 (I1010), was also used with and without PEPQ. The effect of GA concentration on PE properties was also examined between 0 and 1000 ppm. The processed polymer samples were characterized using various techniques, including spectroscopy (FT-IR), rheological (MFR), residual thermooxidative stability (OIT), and color-determining measurements. To prove the UV-stabilizing effect of gallic acid, the samples containing phenolic antioxidants (I1010 and gallic acid) combined with PEPQ were aged in a UV chamber for 42 days. During aging, samples were frequently examined using the above-mentioned methods.

During high-temperature extrusions in an oxygen-poor environment, gallic acid proved more effective than the I1010 industrial stabilizer. Although GA was also found to have excellent efficiency in an oxygen-rich environment, according to the residual stability measurements (OIT), I1010 provided longer OIT for PE. The experiments carried out as a function of concentration revealed that GA is already highly effective at low concentrations. PE stabilized with gallic acid proved more resistant to UV light than that processed with I1010. Compared to the OIT values of the sample containing I1010 and PEPQ, which dropped to almost zero after 27 days of aging, the OIT of the sample prepared with GA+PEPQ was 30 min after 42 days of aging. Natural antioxidants often discolor polymers quite strongly, which might hinder their application in some areas. GA also gives PE a light brownish color, but the extent of discoloration is smaller than in the case of some other natural antioxidants, such as quercetin or curcumin [2].

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Properties of cast polyurethanes synthesized from modified bio-based triisocyanates

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Keywords: bio-based monomers, isocyanate, polyurethane, sustainable production

Polyurethanes (PUs) are a very important group of polymer materials. Due to the possibility of their production in the form of foams, elastomers, coatings, adhesives, and fibers, PUs have been used in a wide range of applications. They are commonly synthesised from polyols and isocyanates, from which various type of polyols from natural origin are now available in the market. The development of bio-based isocyanates it's really important if we want to make these materials more sustainable by using less petrochemicals and reducing the environmental impact [1]. The chemical modification of bio-based isocyanates is promising methodology to tailor their properties towards monomers for polyurethanes characterized by desired features [2,3].

In this study, a series of modified bio-based triisocyanates was obtained by selectively blocking one NCO group of a PDI-trimer using bio-methanol, ethanol and butan-1-ol as blocking agents. The resulting blocked isocyanates were used to obtain cast polyurethanes. Moreover, bio-based poleseter polyols and glycols were used. Obtained materials were next characterized using Fourier-transform infrared spectroscopy (FTIR) and nuclear magnetic resonance (NMR) spectroscopy to confirm their chemical structure. Thermal stability was evaluated through thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). The influence of the modified bio-based isocyanate on the structural and thermal properties of the obtained polyurethanes is discussed, providing insight into their potential applications in sustainable materials preparation.

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Modeling and predicting of nucleation efficiency based on matching lattice dimensions in isotactic polypropylene

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Keywords: crystalline polymers, nucleation, polypropylene

Our work reports a quantitative correlation between the lattice dimensions and nucleating efficiency of additive materials in isotactic polypropylene. The strong correlation is used to build an empirical model, which can predict the possible nucleation efficiency of a material with known crystalline lattice dimensions in isotactic polypropylene. The efficiency of the nucleation is characterized by differential scanning calorimetry (DSC) and thermooptical microscopy (TOM). The crystalline lattice dimensions of all studied materials were collected from existing databases and relative matching parameters were calculated from the comparison of lattice parameters of iPP and the selected additives. To cover wide range of structural matching, additive materials with relatively different lattice parameters compared to those of iPP were also studied. The matching dimensions in different directions are handled as independent parameters and the prediction model is built up by nonlinear regression analysis on the correlation between the dimensional parameters and the nucleation efficiency. The results clearly indicate the strong correlation between the dimensional matching and nucleating efficiency of the additives, and the prediction of efficiency also can be done with good accuracy. Moreover, the correlations obtained in this study revealed that structural mismatch larger than 1 Å is usually enough to eliminate nucleating efficiency of any additive. Based on the results presented in this work demosntrate clearly that investigation of lattice dimensions is a useful and versatile method to search possible new nucleating agents for iPP and such kind of modeling can be very useful in the development of nucleating agents for crystalline polymers.

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Crystallization behavior of Poly(3-hydroxybutyrate) systems incorporating ATBC plasticizer and mesoporous silicas, neat or modified with ATBC

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Keywords: PHAs, plasticization, crystallization

The global accumulation of petroleum-based plastics has reached very critical levels, persisting in ecosystems for centuries and threatening terrestrial and marine life through microplastic contamination. Biodegradable polymers emerge as promising alternatives to mitigate this crisis. Among others, polyhydroxybutyrate (PHB) offers its complete microbial decomposition within months under natural conditions [1-2] after its shelf life. However, a widespread application is limited by its inherent brittleness and crystallization kinetics, which hinder its industrial processing.
Various strategies have been proposed to address these limitations, including the incorporation of nucleating agents, plasticizers, or both; blending PHB with other polymers; and the use of suitable fillers [3].

This study investigates the effects of acetyl tributyl citrate (ATBC), employed as plasticizer, and mesoporous silica particles, neat or modified with ATBC, on improving PHB's crystallization behavior and mechanical properties. Studied materials, prepared by melt extrusion, consisted in: (a) binary compounds of PHB with different contents of ATBC; (b) a binary composite based on PHB with a given amount of mesoporous silica particles (5 wt.%); and, (c) ternary systems of PHB with mesoporous silica particles functionalized with the same ATBC contents added in the binary compounds. Then, films were prepared by press molding and cooled between cold plates refrigerated with water. The crystallization kinetics, thermal properties, and mechanical characteristics of the resulting materials were thoroughly examined.

Thermogravimetry is employed in addition to determine the thermal stability of all of materials to confirm the accurate content of the minor components into the different systems. Calorimetric analyses reveal that ATBC addition delays crystallization, with this effect becoming more pronounced at higher plasticizer amounts. Moreover, melting temperatures appear at lower temperature as decreasing the ATBC content. Mesoporous silica particles, acting as nucleating agents for PHB ordering, shift crystallization temperature to slightly higher values. In composites containing the hybrid plasticizer-silica particles, crystallization occurred slightly faster than that in the binary composite due to the competing effects of nucleating action played by the mesoporous silica and plasticizing role of ATBC. In relation to preliminary mechanical response it should commented that microhardness values significantly decrease with incorporation of the ATBC plasticizer, specially when silica particles are decorated with ATBC.

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Melt memory effect in semicrystalline polymers

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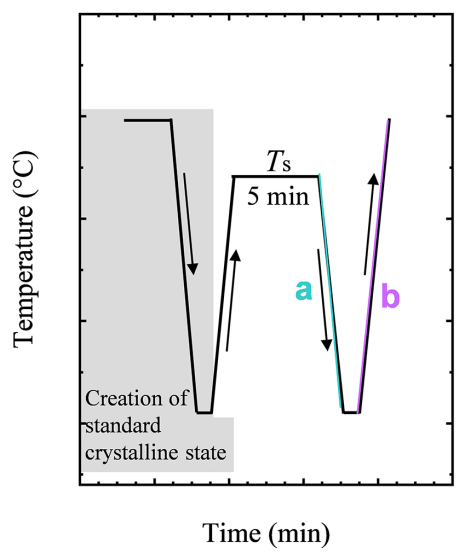
Keywords: polymers, melt memory, self-nucleation

The 70% of commercial polymers are semicrystalline. These polymers are usually processed in the melt and when they cool down they solidify crystallizing. Therefore, during manufacturing crystallization is important since it can determine the time needed to solidify or the temperature at which solidification has finished. The process of crystallization occurs via nucleation and growth. Although both steps have been widely studied in literature, there are still some unknown aspect regarding nucleation. Indeed, it is possible to increase significantly the number of nuclei by heating the material to temperatures below the required ones to remove the thermal history. In that way, some self-nuclei can survive which act as nuclei. In the subsequent cooling those self-nuclei will accelerate the crystallization process and the polymer will crystalize at higher temperatures than the standard crystallization temperature. This increase in the crystallization temperature is displayed even if according to the Differential Scanning Calorimetry (DSC) there are no crystal fragments. This effect is known as melt memory effect and it is very relevant since it could reduce the processing time and the cost of the manufacturing process.

To study melt memory effect self-nucleation thermal procedure is applied. In the first step the material is completely melted, then it is cooled down at a certain rate obtaining a standard crystalline state. The sample is then heated to a selected self-nucleation Ts temperature and kept at this temperature for 5 min. Then the sample is cooled down and heated again at a certain rate. Analysing the a) cooling and b) heating scan it is possible to determine whether the sample displays melt memory effect or not.



Although melt memory has been known for decades that factors that impact this effect have not been studied in detail. One interesting aspect is to elucidate the role of high cooling/heating rates and short times, which is relevant from an industrial point of view. To address this issue fast scanning calorimetry (FSC) has been employed. Then the impact of chemical and physical parameters on the melt memory effect have been studied designing carefully appropriate polymer systems. The role of intermolecular interactions and functional groups

has been studied studying a series of polyesters, polyamides, polyethers or polyester amides. This has allowed to establish a correlation between the intermolecular interactions and the melt memory effect. More recently, the role of molecular weight has been investigated considering a wide range molar mass. The studies with polyethylene oxide with 0.4-900 kg/mol has allowed to ascertain separately the impact of entanglements and extended vs folded chain crystals. The work demonstrates that melt memory originates from topological constraints.

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Curing modeling of an amine-based epoxy resin system

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Keywords: epoxy, curing, differential scanning calorimetry (DSC), rheometry, kinetics modelling

During curing process, epoxy resins form a solid, three-dimensional cross-linked network by reacting with a hardener [1]. The properties of the final product strongly depend on the degree of crosslinking. For this reason, modelling of the reaction kinetics plays a decisive role in predicting cure monitoring as it relates the degree of conversion to the reaction time and/or temperature [2].

An essential aspect to consider when conducting kinetic analysis is vitrification. This transition happens when the glass transition temperature of the system, that increases with increasing degree of cure, reaches the material temperature [3]. It may take place when the reaction occurs at low heating rates or during isothermals, and results in a strong decrease in the reaction rate [1,2].

In this work, the curing reaction of an amine-based epoxy resin is investigated with two different methods: differential scanning calorimetry (DSC) and rheometry. Measurements are performed at different heating rates between 0.1 K/min and 10 K/min. The resulting curves of the heat flow (DSC) and the complex shear viscosity (rheometry) are used to model the reaction rate during complete curing by means of the Kinetics Neo software (NETZSCH-Gerätebau GmbH, Germany).

An Arrhenius model with two successive steps is created to describe the reaction rate over complete curing. The first step is a simplified Kamal-Sourour reaction, the second one an n^{th} order reaction. This model is applied for DSC curves as well as for rheological curves. Additionally, vitrification is characterized for the heat flow curves. For that, the Williams-Landel-Ferry equation is used for temperatures close to the glass transition temperature.

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T22: Pyrolysis

Investigation on pyrolysis of waste printed circuit board: kinetic analysis, product characterization and economic analysis

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Keywords: kinetic analysis, pyrolysis, response surface methodology, waste printed circuit board

In recent years (2010 – 2022), E-waste generation has surpassed the recycling rate by a factor of five [1]. The waste printed circuit board (WPCB) is a suitable candidate for urban mining because of the presence of metals. WPCBs also consist of non-metallic fractions, which are often discarded because of their lower market values. The key challenge faced during WPCB recycling is its complex mixture of materials (metals, polymers and ceramics). Hence, a systematic resource/material recovery approach must be designed. The current work examined direct pyrolysis (without prior removal of metals), followed by the recovery of metals and glass fibers as a potential route for material recovery from WPCB. WPCBs from computer systems were collected, and the bare boards were obtained by removing the economic components mounted on them. The bare WPCBs were pulverized for characterization and experimental purposes. The material characterization techniques include proximate, CHNS, XRF and FTIR analyses. The thermal degradation behavior from 30 to 1000 °C was analyzed using TG-DTG at the heating rates of 5, 10, 20 and 50 °C min^{-1} in nitrogen environment. The kinetic study was performed on TG-DTG data for the determination of the kinetic triplets: activation energy (*E*), reaction model (*f(α)*) and pre-exponential factor (*A)* using isoconversional methods (Friedman, FWO, KAS and Starink), Criado master plot, and constable plot, respectively. The suitability of the developed models was validated by reconstruction of the conversion profiles and estimating the errors. The Starink model was found to be the best fit and the distribution of activation energy values over conversion scale (E_α) ranged from 126.6 – 142 kJ mol^{-1}. The reaction model F1 followed the decomposition with average value of *A* as 8.50×10^9 s^{-1} [2]. Further, the lab-scale pyrolysis experiments were designed using a face-centered central composite design of response surface methodology (RSM) to obtain the optimized parameters (temperature (X), heating rate (Y) and hold time (Z)) to produce maximum oil and minimum char yields (wt%). The optimized conditions (X = 500 °C, Y = 30 °C min^{-1} and Z = 156 minutes) resulted 75.70% char, 7% oil and 17.30% gas yields [3]. The NMR (^1H and ^{13}C), GC-MS and bomb calorimeter of obtained liquid samples showed that the oil is rich in aromatic content (phenolic) and has a calorific value of 34 MJ kg^{-1}. The char characterization using XRF, CHNS and FESEM analyses proved its enrichment in metals and ceramics. The gas composition analysis using GC-TCD and GC-FID showed the presence of H_2, CO, CO_2 and C_1-C_4 gases. The glass fibers and the metals can be separated from char for their application in various fields. Oil and gas can be used as energy resources. Considering these potential applications of the product fractions, economic analysis was performed. The economic parameters- capital cost, operating cost, payback period, and minimum sell-

ing price of oil- were estimated, and a cash flow analysis was performed. The current study shows a detailed investigation on the thermal degradation characteristics of WPCB by means of direct pyrolysis for complete recovery of valuable resources.

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Pyrolysis of waste rubber into sustainable biofuels using solar energy

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Keywords: pyrolysis, solar energy, waste rubber, bio-oil, bio-char yield, environment

The increasing worldwide demand for energy and the dwindling supply of fossil fuels have exacerbated the need for alternative energy sources. Waste rubber plays an important role in addressing present and future energy concerns, as well as meeting the growing need for sustainable energy sources. Besides, it addresses an environmental challenge when reused, and disposal decisions are avoided instead. Pyrolysis of discarded rubber presents a promising approach for generating sustainable energy. This study investigated the effect of temperature during the pyrolysis process on yield (syngas, bio-oil, biochar), physicochemical qualities, and energy production. This was accomplished using a solar-powered pyrolysis apparatus, and the feedstock was waste rubber with particle sizes ranging from 0.01 to 0.1 mm. Experimental and thermodynamic evaluations were carried out at temperatures ranges of 300 to 600°C, with heating rates of 10°C per minute. The results showed that increasing the pyrolysis temperature increased the bio-oil and syngas yields while decreasing the solid yield. The maximum biochar yield (32%) was achieved at 300°C. Furthermore, bio-oil yield reached 45% for particle sizes less than 0.01 mm, while syngas production reached 15% at 600°C. The produced bio-oil showed an average viscosity of 2.56 mPa·s and a density of around 1.07 g/cm³ under all circumstances. Chemical and physical parameters were determined using FTIR, GC-MS, FESEM, and EDX, which revealed the presence of CO, H_2, CH_4, and CO_2.

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Eco-efficient thermal conversion of plastic waste into hydrogen fuel and carbon additives: a life cycle perspective

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Keywords: thermal conversion, waste upcycling, hydrogen production, life cycle assessment

The escalating crisis of plastic waste accumulation presents significant environmental and economic challenges globally. Traditional disposal methods such as landfilling and incineration not only degrade the environment but also overlook the potential value of plastics as resources. This review explores the thermal conversion of plastic waste into hydrogen fuel and carbon additives, offering a sustainable alternative that promotes the principles of the circular economy. A comprehensive life cycle assessment (LCA) of thermally converted plastic waste to hydrogen fuel and carbon additives is presented, analyzing the environmental impacts and economic viability of transforming plastic waste through advanced thermal technologies such as pyrolysis and gasification. The paper highlights advancements in thermal conversion techniques that optimize the yield and quality of hydrogen and carbon products, suitable for use in internal combustion engines and other industrial applications. By integrating innovative technologies such as machine learning, these thermal processes can be enhanced for better scalability and efficiency, facilitating real-time process adjustments and optimizing operational parameters to reduce energy consumption. However, implementing these technologies faces challenges such as high initial capital costs, technological complexities, and the need for regulatory support. The study discusses policy implications and the need for supportive regulatory frameworks to foster the adoption of thermal conversion technologies. Future research should focus on improving the environmental footprint of thermal processes, enhancing system integration, and scaling up operations to industrial levels, thereby advancing the field and providing deeper insights into the broader implications of adopting such technologies.

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A model to estimate the flash point of binary mixtures of ionic liquid and solvent

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Keywords: flash point, ionic liquids, binary ionic liquid + solvent mixtures, flash point prediction

Potential applications of ionic liquids (ILs) in chemical processes commonly involve mixing with flammable solvents. However, there is a lack of flammability data on mixtures of ionic liquid (IL) and solvent in the literature to prevent fire and explosion hazards. Also in the authors' literature review, no flash point prediction models were developed or applicable for IL + solvent mixtures. This study intends to develop a model to estimate the flash point of binary mixtures of ILs mixed with solvents. The model was developed based on the basic theory of the flash point of mixtures and the attribution of IL flammability to their decomposition. [C_6mim][Cl] + methanol/ethanol and [Emim][$EtSO_4$] + methanol/ethanol were selected as examples to validate the proposed model. Since the basis of the model development is related to the decomposition of ILs, the required activation energy for IL decomposition was estimated based on the mass loss rate from thermogravimetric analysis. The results demonstrate that model predictions agree well with experimental data across the entire composition region, with flash point deviations of 5.2°C – 8.3°C when estimating solvent nonideality using the NRTL model, while the size of the flash point range for the studied mixtures is 142.2°C – 165.4°C. The exception is the prediction for [C_6mim][Cl] + ethanol based on NRTL BIPs of Carvalho et al. (2013), with a deviation of 18.4°C. For low IL compositions with flash point temperatures well below the IL flash point, a previously developed binary aqueous–organic solution model provides a good description of the measurements.

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Pyrolysis as a valorization strategy for otr mining tires: experimental study and kinetic modeling

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Keywords: pyrolysis, thermal decomposition kinetics, thermogravimetric analysis (TGA), OTR mining tires, proximate analysis

Pyrolysis is a promising technology for the valorization of polymeric waste, allowing the conversion of complex materials into high value-added products. In Latin America, the management of off-road (OTR) mining tire waste represents a significant environmental challenge. According to Martínez [1], the region generates millions of tons of waste tires annually, with a low recycling rate and inadequate final disposal contributing to pollution and public health problems. These tires, used in large-scale mining equipment, have diameters greater than 26" and are made of resistant materials that hinder their natural degradation. Pyrolysis emerges as a viable alternative to transform these wastes into useful products, contributing to the reduction of environmental impacts and promoting a circular economy. In this study, the pyrolysis of OTR mining tires from a recycling plant was evaluated, reduced to particles smaller than or equal to 5 mm. The process was carried out in a laboratory-scale fixed-bed reactor under a nitrogen atmosphere, at temperatures of 500, 600 and 700 °C. The fractions of solid products (20-30%), condensable liquids (60-75%) and non-condensable gases (5-15%) were quantified, in addition to characterizing the raw material to establish its moisture content (2%), volatile matter (87%) and ash (11%). Additionally, thermal degradation kinetics were studied by thermogravimetric analysis. (TGA) at different heating rates (10, 25, 40 and 60 °C/min) in a nitrogen atmosphere. The Friedman isoconversional method was applied to determine the apparent activation energy, which varied between 150 and 180 kJ/mol, and the reaction model was identified by using master plots. The results showed that the decomposition mechanism follows a two-dimensional diffusion model, with a pre-exponential factor of 1.5 × 10^9 s^-1. These values are within the range reported in the literature for the thermal decomposition of complex polymeric materials [2, 3]. The experimental and theoretical data showed an excellent correlation, validating the proposed kinetic model. Pyrolysis of OTR mining tires proved to be an effective strategy for obtaining valuable products, such as solid carbon, oils and combustible gases, which opens opportunities for its implementation on an industrial scale. These results provide key information for the design and optimization of pyrolysis processes, contributing to the sustainable use of mining tire waste and the generation of products with potential added value. Future studies could focus on the detailed characterization of the products obtained and on the economic evaluation of the process.

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Optimizing thermal recycling of glass fiber-reinforced polymer composites

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Keywords: glass fiber, epoxy, thermal recycling, pyrolysis, oxidation

Glass fiber-reinforced polymer (GFRP) composites are widely used in industries such as wind energy, automotive, consumer goods, and construction due to their superior mechanical properties [1]. The increasing use of GFRP composites has led to significant waste generation, particularly from the wind energy sector, where the decommissioning of turbine blades is expected to drive a substantial increase in GFRP waste by 2030 [1]. With wind energy projected to supply 50% of EU electricity by 2050 and the Asian market expected to grow ninefold, the challenge of managing GFRP waste will become even more critical [1]. However, the disposal of GFRP at end-of-life (EOL) presents significant environmental challenges, hence necessitating the development of sustainable recycling methods for fiber recovery. Current recycling approaches include mechanical, thermal, and chemical methods. This study focuses on thermal recycling as a viable strategy for GFRP recovery, evaluating three distinct process routes: (i) pyrolysis followed by oxidation, (ii) pre-treatment before pyrolysis and oxidation, and (iii) direct oxidation.

Based on thermogravimetric analysis and data from the literature, pyrolysis was carried out at 500˚C with a dwell time, yielding fibers with residual pyrolytic carbon. Oxidation experiments were performed at 500˚C for 30 and 60 minutes to remove this residue, with complete removal achieved at 60 minutes. A major challenge in thermal recycling is the loss of fiber tensile strength at elevated temperatures. To mitigate this, a pre-treatment step was introduced, involving magnetic stirring in a 20% (w/v) ethanol-$ZnCl_2$ solution at 75˚C for 2 hours. This approach reduced the pyrolysis temperature by approximately 90˚C, with optimized conditions of 350˚C and a dwell time of 20 minutes. However, despite lowering the pyrolysis temperature, the catalyst system was ineffective in removing carbon residues, necessitating oxidation at 500˚C for complete residue removal.

Given that oxidation was essential to complete the removal of carbon residues, direct oxidation of GFRP specimens was investigated at temperatures between 400 and 550˚C.550°C. Below 500˚C (400, 450, and 475˚C), no residue removal was observed even after 300 minutes. At 500˚C, clean fibers were obtained within 60 minutes. To assess the impact of temperature and dwell time on fiber strength, additional studies were conducted at 500˚C (120 min) and 550˚C (60 min). The highest restoration of tensile strength (26.81%) was observed at 500°C for 60 minutes, whereas increasing the temperature to 550 ° C reduced residue removal time but severely degraded the fiber strength (5.24% restoration). The literature reports tensile strength recoveries of 20–40% under similar conditions [2], highlighting the

challenge of balancing residue removal with fiber integrity. Further research into the refinement of the oxidation process, including catalyst utilization and controlled atmospheres, is crucial to enhancing the quality and mechanical performance of recycled fibers.

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Thermal conversion of plastic waste into fuels and lubricant additives for hydrogen internal combustion engines: a systematic review

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Keywords: hydrogen internal combustion engine, thermal conversion; plastic waste management; waste to wealth

The escalating accumulation of plastic and microplastic waste underscores the urgent need for innovative approaches to convert these pollutants into valuable products, such as battery electrodes, carbon nanomaterials, membranes, and graphene. Thermal conversion processes, including pyrolysis, plasma-catalytic pyrolysis, and graphitization, have emerged as effective pathways to transform plastic waste into fuels and lubricant additives, particularly benefiting hydrogen-powered internal combustion engines (ICEs). This review provides a comprehensive discussion on the production of fuels and hydrogen via thermal conversion processes, emphasizing their applications in hydrogen ICEs. A critical examination of structural transformations during these processes is presented, highlighting their impact on engine performance and longevity. Among various thermal conversion techniques, steam gasification of blended plastic waste with a CaO catalyst demonstrated a high hydrogen fuel yield of 104 mmol/$g_{plastic}$. Meanwhile, pressurized batch pyrolysis and batch pyrolysis exhibited superior liquid fuel and polymer oil production efficiencies, achieving yields of 97wt. % and 96.7 wt. %, respectively. Beyond fuel production, this review underscores the significant potential of thermal conversion processes for producing lubricant additives from plastic waste. The conversion pathways are categorized into direct and indirect thermal conversion methods, each offering distinct advantages for lubricant performance enhancement. In direct thermal conversion, processes such as pyrolysis, flash joule heating, and graphitization transform plastic waste into carbon-based materials, including carbon nanomaterials, graphite, and graphene. These carbon derivatives are highly valued for their superior tribological properties, which significantly enhance lubricant performance by reducing friction, minimizing wear, and improving overall mechanical efficiency. The unique structural characteristics of these materials, such as high surface area and thermal conductivity, contribute to their ability to maintain stable lubrication under extreme operating conditions. On the other hand, indirect thermal conversion methods produce a diverse range of functionalized

hydrocarbons, nitrogen-enriched carbon additives, and other high-value compounds. These derivatives play a crucial role in improving lubricant characteristics by enhancing viscosity stability, oxidation resistance, and thermal performance. Functionalized hydrocarbons can act as effective dispersants and anti-wear agents, while nitrogen-enriched carbon materials improve thermal conductivity and anti-corrosion properties. Together, these direct and indirect conversion pathways demonstrate the versatility of thermal conversion technologies in creating advanced carbon-based additives that can optimize the performance and longevity of lubricants, particularly in hydrogen internal combustion engine applications. In addition, this review highlights the emerging potential for converting microplastic waste into carbon materials or carbon nanotubes. Due to their large surface area and unique physicochemical properties, these materials are promising candidates for lubricant additives

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Online qualitative and quantitative study of pyrolysis products from tobacco granules: the influence of drying process

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Keywords: granule-based HTP, TG-FTIR-MS, PI-TOFMS, release pattern, gas/particulate distribution

The study focuses on the development and application of tobacco granule in heated tobacco products (HTPs). Tobacco powder was mixed with the liquid materials, and an extrusion molding process was used to prepare the granules. The wet granules were then dried using three processes, namely blast drying (bd), microwave drying (md), and fluidized - bed drying (fd), to prepare granules with different physical properties. Particle size distribution, specific surface area, porosity, microscopic surface morphology, and functional group features were tested for the three samples. After that, pyrolysis tests were conducted using a TG-FTIR-MS system. TG and DTG results showed that the pyrolysis process of the granules occurs in three stages: the low-temperature stage (below 150°C) is primarily the evaporation of water and volatile components; the medium-temperature stage (200°C to 400°C) involves the thermal decomposition of organic components; and the high-temperature stage (above 500°C) shows consistent non-volatile residue. Online FTIR and mass spectrometry analyses reveal that the major release of emitted gases occurs above 200°C and differed among the three samples. Glycerol (VG) shows a primary release peak at lower temperatures under fluidized bed drying, while propylene glycol (PG) continues to release significantly at higher temperatures. The notable release of nicotine occurs post-combustion, indicating its release capability under pyrolytic conditions is weaker than in ignited states. Additionally, this study identifies other significant substances in the emitted gases, categorized into those released before the combustion point, after the combustion point, and those released at both times, encompassing various organic compounds. Granules were then transformed into cigarette for online quantitative analysis using a novel vacuum ultraviolet (VUV) photoionization time-of-flight mass spectrometer (PI-TOFMS). The on-line analyzer was able to detect a great number of mass peaks, including nicotine, VG and PG *etc* in the particulate phase, and flavor components such as 2,3-Butanedione and triethyl citrate in both gaseous and particulate phases. In particular, some short-lived intermediates such as ethenol and propen-2-ol from pyrolysis of the tobacco granules were observed and identified on-line. Nicotine, VG and PG were quantified with a high time resolution of 0.5 s using their standard calibration curves established with PI-TOFMS. The time-resolved evolving mass profiles of Nicotine, VG and PG were obtained in near real-time, as well as Nicotine release rate within a single puff for the first time.

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T23: Theory and instrumentation

Quebec Centre for Advanced Materials (QCAM) – the power of hyphenation

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Keywords: facility, instruments, thermal analysis, TGA-FTIR-GC/MS, EGA

The Quebec Centre for Advanced Materials (QCAM) is a strategic interuniversity cluster funded by the Fonds de recherche du Québec – Nature et Technologies, dedicated to advancing cutting-edge research in materials science. With more than 100 regular members and over 1,000 graduate students across 16 institutions, QCAM stands as one of North America's leading centres for materials research. Its members and external collaborators have access to a vast array of advanced equipment, distributed across 16 affiliated facilities. The skilled research professionals at these locations play a crucial role—not only by delivering top-tier technical support, but also by mentoring and sharing their expertise with the next generation of scientists. This presentation highlights the Thermal Analysis and Spectroscopy (TAS) Lab, one of the satellite facilities of QCAM, located in the chemistry department at McGill university, featuring the PerkinElmer hyphenation system. As an example, we present the investigation of isocyanide complexes, featuring a key strength of thermogravimetric analysis — the ability to readily integrate with complementary techniques.

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Design an embedded vest system for human being real time vibrations measurement

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Keywords: biomechanics, human being, measurements, vibrations

Mechanical machinery and transportation vibrations can harm health. Certain vibrations might diminish comfort and increase the risk of spine fractures and lower back pain. Researchers have shown that investigating biodynamic response helps minimize vertical vibration-related injuries by revealing their impacts on the body. In order to assess vibration threats in a variety of applications, this paper details the design of an embedded system for a wearable body vest that records responses at critical locations on the human body. It is designed to employ 801S vibration sensors, which are dispersed across the body's upper and lower regions. These sensors are linked to an Arduino board, which can process the signals from the sensors, alter them, and then display them in an understandable manner for simple usage. To increase human safety, the design prototype takes into account various kinds of mobility and mechanical equipment. This is crucial because over time, vibrations from these sources may cause damage to the body's joints. Numerous everyday actions, such as operating heavy machinery, driving a car, and riding the bus, can cause these vibrations. The four investigations employed an electrical jackhammer, a bus, a car, and a vibrating chair. According to the results, the greater vibrations are more prevalent in the lower backbone of the body than in other joints, gradually diminishing in intensity as they ascend up the spine. Furthermore, the results revealed that vibrations in the lower part of the body tend to focus near the knees. While the wrist, elbow, and shoulder joints have been shown to have the largest concentration of vibrations. the lower body has not been subjected to as much. It has been concluded that the higher frequency outputs were focused along the spine and on the chest. Consequently, it is difficult to ignore how vertical vibrations affect the human body in any application.

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T24: Thermal conductivity

Correlation between thermal and optical properties in znmnse mixed crystals grown by the bridgman technique

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Keywords: semiconductor alloys, crystal growth, photopyroelectric calorimetry, thermal conductivity, lattice disorder

Broadband solid solutions of II-VI compounds are of significant interest both for theoretical exploration and for practical applications in modern optoelectronics. However, their physical properties remain largely unexplored due to the complexity of their preparation technology. Despite this, II-VI mixed crystals remain important for contemporary electronics, optics, and spintronics, as they offer the possibility of manipulating material properties such as energy gap and lattice constant.

Zinc manganese selenide, a type II-VI semiconductor with a tunable bandgap, is attracting considerable interest due to its diverse applications, including nuclear radiation detectors and industrial process monitoring. This study investigated the thermal and optical properties of $Zn_{1-x}Mn_xSe$ ternary semiconductors obtained by the vertical Bridgman-Stockbarger growth method over a manganese content range from 0 to 0.42. The composition of the samples was determined using the energy dispersive analysis (EDS) technique. X-ray diffraction (XRD) was used to characterize the crystalline structure of the material. The results revealed a phase transition, with a zinc blende structure observed for $x \leq 0.15$ and a hexagonal structure for $x > 0.15$.

Ellipsometry was utilized to measure the bandgap energy and refractive index of the studied samples. The experimental findings showed that the bandgap energy of the ZnMnSe samples varied from 2.66 eV for $x = 0$ to 2.8 eV for $x = 0.42$. Measurements performed within the spectral range of 0.6 to 6 eV revealed that increasing the manganese concentration to 0.42 results in an increase of approximately 0.15 eV in the fundamental energy gap at room temperature. These results highlight the significant influence of manganese incorporation on the electronic structure of the material. The empirical relation between band-gap energies and composition ratio accorded with a bowing parameter b ($b = 0.53$ eV).

Thermal studies were also carried out using the photopyroelectric calorimetry (PPE) technique [1]. The thermal diffusivity and effusivity values were extracted from the experiment, allowing the calculation of the specimens' thermal conductivity using the Adachi model [2].

The results show that the energy gap increases with the increase in Mn concentration. Moreover, the thermal diffusivity and conductivity of the studied materials decrease as the Mn content in $Zn_{1-x}Mn_xSe$ increases. Based on these measurements, it can be concluded that the incorporation of Mn into ZnSe crystals has a significant impact on their optical and thermal properties These results provide valuable information on the optical and thermal properties of $Zn_{1-x}Mn_xSe$ compounds and contribute to a better understanding of their behavior in different fields of application.

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Thermal modelling of a suspended microheater surrounded by air and hydrogen

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Keywords: thermal conductivity sensor, 3 omega method, suspended microheater, helium concentration, thermal modelling

Hydrogen possesses a thermal conductivity approximately seven times higher than air, allowing the hydrogen concentration in air to be deduced through thermal conductivity measurements of the gas mixture. Owing to this unique physical property, thermal conductivity-based sensing methods are widely adopted in applications requiring high measurement accuracy, a straightforward sensor configuration, and a broad concentration range. However, a primary challenge persists in detecting hydrogen at low concentrations, particularly below a few percent. Conventional thermal conductivity sensors typically lose sensitivity in low-concentration regimes, motivating the need for sensor designs to mitigate this limitation. A promising approach involves using 3-omega sensors that integrate microheaters fabricated on substrates with low thermal conductivity or designed as suspended bridge structures. This design strategy enhances sensitivity by reducing parasitic heat losses through the substrate, enabling more accurate measurements of minor changes in the thermal conductivity of the surrounding gas. Previous studies have demonstrated that suspending the microheater greatly diminishes conduction to the substrate, thereby improving the sensitivity to low hydrogen concentrations [1]. This study presents a theoretical and experimental investigation aimed at characterizing a suspended microheater-based 3-omega sensor for accurate hydrogen detection in air. The sensor operates by inducing an AC Joule heating in a microheater. The thermal conductivity of the ambient gas strongly influences these temperature oscillations. By comparing measured temperature oscillations under vacuum, pure air, and air–hydrogen mixture environments, we constructed a heat transfer model to quantify conduction, convection, and radiative losses. Under vacuum conditions, we established a baseline for radiation heat transfer and conductive leakage through the supporting bridge structure. When various mixtures of air and hydrogen were introduced, gas-phase conduction and convection were incorporated into the model as additional thermal resistances. We validated our theoretical model with experimental measurements. The comparisons confirmed that the model accurately predicts the sensor's thermal response across varying hydrogen concentrations. The sensor was found to be capable of detecting hydrogen concentrations as low as approximately 0.5 vol.% in air. Furthermore, we explored potential avenues for improving detection limits. One strategy involves refining the suspended bridge geometry to minimize conduction pathways within the sensor, while another entail optimizing the thin-film heater's dimensions to ensure higher temperature responsiveness. These findings underscore the promise of suspended microheater-based 3-omega sensors in broadening the operational window for hydrogen detection. Given the growing importance of hydrogen in diverse industries, this research lays a foundation for more robust, sensitive, and scalable solutions to hydrogen leak detection and real-time monitoring in safety-critical environments.

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T25: Thermal hazards, lifetime prediction

Study on thermal stability of ionic liquid [bmim] [tfo] in different atmospheres

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Keywords: ionic liquids,TGA/DSC, 1-Butyl-3-methylimidazolium triflate [Bmim][TFO], thermal stability

Ionic liquids (ILs) are a class of molten salts characterized by their organic cation-anion combinations, where the cationic species can be paired with either organic or inorganic anions. Usually, they are classified into four main categories based on their cationic architecture: pyridinium salts, pyrrolidinium salts, imidazolium salts and quaternary ammonium salts. Earlier scientific studies believed that the ionic nature of these substances resulted in negligible vapor pressures, contributing to their inherent non-combustibility. However, more recent research has shown that the flammability of ILs is mainly due to the combustion of gaseous decomposition products rather than direct ignition of their vapors [1]. Traditionally, the thermal stability characteristics of ILs have been evaluated in the inert gas atmosphere, but, some recent studies have shown that ILs may have different reaction mechanisms under nitrogen and air atmospheres. It has been reported that some ILs undergo an endothermic reaction in a nitrogen atmosphere, but an exothermic reaction in an air atmosphere [2]. The ionic liquid 1-butyl-3-methylimidazolium trifluoro-methanesulfonate ([Bmim][TFO]) has been found to have a wide range of applications, including as a fiber catalyst in low temperature pyrolysis, as an electrolyte in fuel cells and as a corrosion inhibitor for CO_2 capture. However, its thermal stability characteristics have been largely ignored when used as battery electrolytes. In this study, thermogravimetric analyzer/differential scanning calorimetry (TGA/DSC) and auto-ignition tester were used to evaluate the thermal stability of [Bmim][TFO] in different gas atmospheres.

The results showed that the DTG curve of [Bmim][TFO] showed peaks at 425°C and 445°C in air atmosphere, which together with the TGA curve indicated that the decomposition reaction could be a two-step reaction. Besides, the residual weight on the TGA curve is 0% in air atmosphere. The DSC curve shows that the first stage is an endothermic reaction (306.2 J/g) and the second stage is an exothermic reaction (-542.8 J/g). Under a nitrogen atmosphere, a peak was observed in the DTG curve, suggesting that the decomposition reaction may be a single-step reaction and the TGA curve showed a residual weight of 4.6%, and the DSC curve indicated that the decomposition reaction was endothermic with a value of 485.2 J/g. Comparing the TGA curves of these two atmospheres, it can be seen that the estimated onset temperature of the first-step reaction in the air atmosphere is approximately the same as that in the nitrogen atmosphere, but there is a significant difference between the residual weights in these two atmospheres. The DSC curve in the air atmosphere indicates

the first-step reaction was endothermic, but the second-step was exothermic. In addition, the residual weight of the TGA curve is 0% in the air atmosphere, it is then concluded that the second-step reaction in the air atmosphere might be the spontaneous combustion of the decomposition products of [Bmim][TFO], which caused the observed heat effects to change from endothermic to exothermic. A subsequent auto-ignition temperature test showed that [Bmim][TFO] auto-ignition occurred at 452°C, the temperature at which the prominent heat release is seen in the DSC curve. The results of this auto-ignition temperature test preliminarily confirmed the above conclusion.

Acknowledgments
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The thermal stability of [PYR14][NTF_2] under different atmosphere

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Keywords: ionic liquid, TGA/DSC, TGA-FTIR

With the increasing global demand for energy, many studies focused to the development of high-efficiency and low-pollution energy storage systems. Among these energy storage technologies, lithium-ion batteries (LIBs) have attracted attention due to their high energy density and wide application in low-power devices. However, the organic electrolyte used in conventional LIBs has the problem of low thermal stability, which leads to safety hazards such as fire or explosion in high-temperature environments. To solve this problem, researchers have started to explore alternative electrolyte materials with higher thermal stability in recent years. MacFarlane et al. found that pyrrole ionic liquids are ideal for replacing conventional lithium battery electrolytes due to their high conductivity and high thermal stability compared to conventional electrolytes [1], however, there is a relative lack of research on the thermal stability of pyrrole ionic liquids. The study of thermal stability is therefore crucial for the practical application of such ionic liquids in battery technology. In this study, we investigate the thermal stability of 1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl) imide ([PYR14][NTf_2]), a widely used pyrrolidinium-based ionic liquid for electrolyte applications. The thermal stability of [PYR14][NTf_2] is analysed using TGA/DSC and TGA-FTIR in both the nitrogen and air atmospheres.

Under nitrogen atmosphere, the estimated onset temperature was observed to be 427.7°C in the TGA curve of [PYR14][NTf_2] and a peak at 453.7°C was observed in the corresponding DTG curve. These observations indicated that the decomposition reaction might be a single step reaction. Moreover, the DSC curve showed the decomposition reaction is endothermic with the heat of 1300.7 J/g. Under air atmosphere, both TGA curve and DTG curve have similar behavior as those under nitrogen atmosphere with the estimated onset temperature and peak temperature were of 418.4°C and 443.5°C for the TGA curve and DTG curve, respectively. However, the DSC curve showed the decomposition reaction is exothermic with the heat of -1639.1 J/g. TGA-FTIR experiments were carried out to investigate whether the different heat effects observed indicate that different decomposition mechanisms occur in different atmospheres. The FTIR spectra were retrieved and compared at the following temperatures: $T_{2\%}$, T_e , T_{peak} and T_{endset} for both nitrogen and air atmosphere. Under nitrogen atmosphere: at 400°C ($T_{2\%}$), a small amount of trifluoromethane and sulphur dioxide appeared, at 441°C (T_e), the concentration of the above products increased, and a small amount of methane and propane appeared, at 459°C (T_{peak}), the concentration of all the above products increased, and at 469°C (T_{endset}), the concentration of all the products decreased. Under air atmosphere: at 384°C ($T_{2\%}$), a small amount of trifluoromethane and sulphur dioxide appeared, and these observations identical to those observed in nitrogen atmosphere, at 436°C (T_e), the products observed were also identical to those observed in nitrogen atmosphere, at 455°C (T_{peak}), in addition to the products observed in a nitrogen atmosphere, small amounts of hydrogen fluo-

ride, formaldehyde and hydrogen cyanide were also observed, and the observed intensities of carbon dioxide, carbon monoxide and water vapour were all increased, at 465°C (T_{endset}), the concentration of gaseous products other than carbon dioxide and carbon monoxide all decreases. As decomposition products observed are different at T_{peak}, which means the reaction mechanism starts to be different for nitrogen and air atmosphere at this temperature. Moreover, the appearance of large amounts of carbon dioxide, carbon monoxide and water vapour implies auto-ignition of the decomposition products in air atmosphere, which is also confirmed from the exothermic phenomenon in the DSC curve under the air atmosphere.

Acknowledgments
The authors would like to thank the Ministry of Science and Technology, R.O.C. for supporting this study financially under grant number: NSTC 112-2221-E-992 -021 -MY3.

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T26: Thermochemistry

Thermodynamic characterization of 2-picolinamide polymorphs

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Keywords: polymorphism, calorimetry, vapor pressure, computational thermochemistry

The physical and chemical stability of organic molecules plays a crucial role in the rational design and development of fine chemicals, such as pharmaceuticals and agrochemicals. Despite the extensive thermodynamic data available, a standardized benchmark for evaluating the equilibrium stability of crystalline polymorphs is still lacking, limiting the validation of computational predictions. In this context, COST Action CA22107 "Bringing Experiment and Simulation Together in Crystal Structure Prediction" (BEST-CSP) aims to establish such benchmarks through collaboration between experimental and computational scientists.

This work contributes to that effort by focusing on the thermodynamic characterization of the polymorphic forms of 2-picolinamide (2-PCA), whose molecular formula is presented in Figure 1. The study targets energetic and structural properties of forms I and II, employing experimental techniques to determine essential data on assessing polymorphic stability.

The experimental approach integrates Differential Scanning Calorimetry (DSC) for the study of phase transitions and of fusion enthalpies, Knudsen Effusion for vapor pressure measurements, and Combustion Calorimetry for the determination of enthalpies of formation. These complementary techniques enable a comprehensive analysis of the thermodynamic parameters, providing insights into the energy of intermolecular interactions and polymorphic stability.

Additionally, theoretical calculations in the gas phase using the G3(MP2)B3LYP composite method and isodesmic reactions were employed to calculate the gas-phase enthalpy of formation of 2-PCA. This approach established a robust thermodynamic cycle, facilitating direct comparison between experimental and computed formation enthalpies and improving the understanding of molecular stability and intermolecular binding forces.

The results revealed a low enthalpy of a crystal-crystal transition, indicating minimal energetic differences between the polymorphs, while similar sublimation enthalpies confirmed comparable molecular packing forces. These findings contribute to the development of benchmark datasets for validating computational models, advancing crystal structure prediction methodologies, and enhancing the reliability of thermodynamic stability assessments.

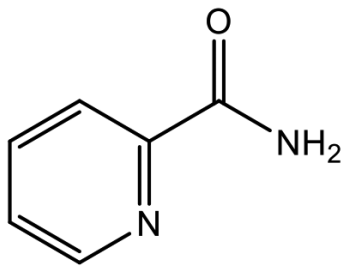

Figure 1. Structural formula of 2-picolinamide.

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Utilization of powdered hydrate salt in vacuumed heat pipes for enhanced solar energy harvesting

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Keywords: heat pipe, salt hydrate, temperature, powder

This study compares the performance of a heat pipe using powdered $MgSO_4 \cdot 7H_2O$ (Magnesium Sulfate heptahydrate) and water as working fluids. To this purpose, a stainless-steel heat pipe is vacuumed and divided into three sections: the evaporator, adiabatic, and condenser sections. The temperature changes, heat transfer, and pressure of the heat pipe with a constant temperature boundary in the evaporator were monitored. To compare the system's performance, two states were investigated: time-on (e.g., during the day when sunlight serves as the heat source) and time-off (e.g., at night). The results demonstrated that there is no significant temperature difference between the inlet and outlet of water in the condenser for powdered $MgSO_4 \cdot 7H_2O$ in the heat pipe during the time-on mode—approximately half that of water—indicating reduced heat transfer efficiency. Although greater thermal resistance was achieved for powdered $MgSO_4 \cdot 7H_2O$ in time-on mode due to the higher temperature difference between the evaporator and condenser, its ability in time-off mode, due to the hydration process, makes it advantageous for applications like solar energy harvesting. Moreover, the operational pressure of $MgSO_4 \cdot 7H_2O$ approaching that of water in a steady-state heat pipe system emphasizes the potential of salt hydrates in improving heat pipe performance, paving the way for further studies in renewable energy technologies.

Mixed cation sulfates as thermochemical energy storage materials

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Keywords: thermochemical energy storage; TGA, DSC, Tutton salt, salt hydrate, solid solution

Energy security is a topic of ever-increasing importance. The harmful effects of greenhouse gas emissions and the resulting dramatic global warming have long been an impetus for reducing fossil fuel dependence, and for many countries, the urgency of the matter has become even more tangible with the war in Ukraine. A key step in the process of decreasing energy dependency is increasing energy efficiency via energy storage and waste heat capture; thermochemical energy storage is a promising solution for these applications, as it offers potentially lossless storage and higher storage densities than sensible or even latent heat storage. Thermochemical energy storage reactions can utilize the reversible thermal decomposition reaction of a material such as a salt hydrate into easily separable products to store energy indefinitely. Salt hydrates that have been extensively researched include readily available salts like the hydrates of magnesium chloride, which can decompose, thereby releasing corrosive hydrogen chloride, and magnesium sulfate, which suffers from sluggish rehydration [1].

The Vienna TCES database inspired us to turn to lesser-known salts, such as the Tutton salts, of which we synthesized and analyzed a solid solution library of 40 mixed Tutton salts $K_2Zn_{1-x}M_x(SO_4)_2 \cdot 6H_2O$ (M = Mg, Co, Ni, Cu) [2]. The compound library displayed several interesting trends: the reaction temperature can be increased nearly linearly by increasing the nickel content, whereas copper decreases the reaction onset temperature. Further work has been conducted on 30 mixed sulfates of the form $M_{1-x}M'_xSO_4 \cdot nH_2O$, and scanning electron microscopy has been conducted to shed light on particle morphology and elemental distribution. Ongoing projects aim at incorporating successful candidate materials in reactors not only for energy storage, but also for use as heat transformers.

Acknowledgments
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TCMs for versatile thermal energy storage – from salt hydrates to oxides

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Keywords: thermochemical energy storage, salt hydrates, metal oxides, metal hydoxides

Thermal energy storage can play a crucial role in supporting the European Union Green Deal via reducing the need of fossil fuels for industrial process heat as well as domestic heating and warm water supply. In contrast to some applications based on sensible heat or latent heat using phase change materials (PCMs) already on the market the principle of thermochemical energy storage based on reversible chemical solid-gas reactions is still at a rather low technology readiness level [1]. However, several classes of compounds have been identified via a systematic algorithmic database search as promising candidates [2]. Among these the salt hydrates represent a peculiar class of compounds we investigated in the last decade. Presenting a few examples of our research the challenges and chances with respect to cycle stability [3] as well as thermal property tuning [4] are discussed. Furthermore, there is another class of compounds using water for a reversible thermochemical energy storage material, *i.e.* the metal oxides being hydrated to metal hydroxides. For example, for medium temperature applications the system $MgO + H_2O \rightleftharpoons Mg(OH)2$ is presented with respect to the performance enhancement we could achieve via Ca-doping [5].

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T27: Fire dynamics (or others for fire safety)

Experimental investigation of pool fire behavior and unburnt gas ignition hazards in a reduced-scale model chamber of chambord castle

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Keywords: pool fire, fire behavior, cultural historic building, reduced-scale, under-ventilated, fire safety

Historic buildings' design restrictions, usage of flammable materials, and limited ventilation make fire safety in historic buildings a major issue. Devastating fire accidents such as the 1989 Chiado fire in Portugal, the 2006 Trinity Cathedral fire in Russia, and the 2019 Notre-Dame fire in France draw attention to the fragility of buildings of cultural legacy. While fire dynamics in confined compartments have been extensively investigated in contexts including nuclear reactors and high-altitude chambers, few studies have been done on fire behavior in historical buildings. This work attempts to address this discrepancy by investigating fire dynamics and related risk in a reduced-scale model of the Queen's Room at Chambord Castle across different combustion regimes.

A 1/8th-scale model replicating a chamber from Chambord Castle was constructed following Froude scaling laws to represent fire behavior accurately. A total of 36 fire tests were conducted using n-heptane as the fuel, with the same initial mass of 200 g, across four pool diameters (13 cm, 16 cm, 20 cm, and 24 cm) and three air renewal rates (10, 20, and 30 ACPH). The study examined key fire behavior parameters, including mass loss rate (MLR), heat flux, temperature distribution, and gas concentrations near the ceiling for oxygen (O_2), carbon dioxide (CO_2), carbon monoxide (CO), hydrogen (H_2), and hydrocarbons (C_xH_y).

The results show that under-ventilated, well-ventilated, and substantially under-ventilated regimes have quite different fire behavior. Combustion stays well-ventilated for small pool fires (13 cm diameter), with continuous MLR following the growth stage and oxygen levels over 10%, so guaranteeing effective burning. Fires enter the under-ventilated regime as the pool diameter increases (16 cm diameter), where oxygen depletion reduces combustion efficiency, hence peaking the MLR early before descending to a lower plateau. However, larger pool fires (20–24 cm diameters) transition into the severely under-ventilated regime, where oxygen supply becomes very insufficient, leading to a continuous decline in MLR and a significant accumulation of unburnt gases. The study also reveals that ventilation rate has a much less pronounced effect on fire behavior than pool size for the chimney-like ventilation configuration of historic buildings. At last, a notable low-frequency oscillation phenomenon [1] is observed in certain configurations, suggesting complex interactions between pressure variations, gas mixing, and fire dynamics in confined spaces. To assess the ignition hazard of unburnt gases, a global risk assessment model was applied [2], considering auto-ignition temperature (AIT) and lower flammability limits (LFL). The 16 cm pool fire at 10 ACPH

remains below the ignition threshold, while the 24 cm fire at 10 ACPH showed a high ignition potential due to its higher concentration of flammable gases and elevated temperatures near the ceiling. These findings highlight the need for optimizing ventilation and monitoring unburnt gases, particularly in severely under-ventilated fire scenarios.

Despite these findings, several important areas remained to be explored: (1) the influence of local turbulence flow and pressure variations on unburnt gas accumulation requires further investigation; (2) an experimental method for accurately mapping the distribution of unburnt gases during combustion is still lacking; (3) future work will focus on detailed numerical simulations and extended experimental studies incorporating different fuel types and depths to enhance the understanding of fire dynamics in heritage buildings and similar enclosed environments.

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Poster Presentations

T01: Bio sciences, including food, soil, textile, wood

Survival and grouth of spirulina platesis cells in a zarrouk's medium where k+ was replased by an equal molar amount of Cs^+ ions, irradiated with Cs137 γ at 180 kGy

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Keywords: spirulina platensis irradiation optical absorption differential scanning calorimetry dsc

Using the DSC and optical studies, it was shown that Spirulina platensis irradiated with Cs137 γ at 180 kGy for 113 days in a standard Zarrouk's alkaline saline aqueous medium under anaerobic and dark conditions at 15 to 18°C, where K^+ was replaced by an equal molar amount of Cs^+ ions, exhibited 95% denaturation of its entire biomass. After recultivation, Spirulina platensis (pre-irradiated with Cs137 γ at doses of 180 kGy) for 14 days in a standard Zarrouk's alkaline saline suspension demonstrated full restoration of its physical, chemical, and biological characteristics. In particularly, $\Delta H_m = 38.85$ J/g, $T_m = 56.5 \pm 0.3$°C, and $\Delta T = 3.8 \pm 0.5$°C, the cell growth increased by 5 %, and the phycobilisome complexes (PBPc) increased by 10 % compared to the normal values. These values were similar to those of freshly cultivated Spirulina platensis, which suggests that it may also survive simultaneous irradiation and high concentrations of Cs^+ (2 mg/mL). This finding is significant as Spirulina platensis could potentially be used as one of the best microalgae in space missions, including those to Mars.

Recent developments in sustainable composting methods for organic fertilizer production from biowaste

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Keywords: biowaste, composting technologies, organic fertilizers, circular economy

The rapid growth of the global population and escalating food production demands have intensified the reliance on chemical fertilizers leading to severe environmental impacts. This review explored sustainable alternatives through the valorization of biowaste into organic fertilizers with a particular focus on composting technologies. The study highlighted the significance of food and agricultural waste as a rich source of nutrients, emphasizing its role within the circular economy framework. Various composting methods including manual (e.g., windrow, bin, and vermicomposting) and automatic (e.g., in-vessel and forced-aerated systems) are critically evaluated based on efficiency, cost, scalability, and environmental performance. Advanced bioreactor designs and operational parameters (e.g., moisture, temperature, C:N ratio, porosity, and pH) are discussed as crucial determinants of compost quality. The study also addressed composting's dual environmental role: mitigating greenhouse gas emissions while enhancing soil health. Life cycle assessment (LCA) approaches were explored to quantify composting's ecological footprint compared to landfilling and incineration. Furthermore, the integration of Artificial Intelligence (AI) and Internet of Things (IoT) technologies is presented as a transformative advancement for real-time monitoring, parameter optimization, and emission control. AI-based models enhance compost maturity prediction, microbial activity tracking, and process automation. Challenges such as odor management, nutrient loss, and system scalability are acknowledged. Overall, this comprehensive review underscores composting as a viable, eco-friendly alternative for managing biowaste and producing high-quality organic fertilizers, fostering sustainable agriculture and climate resilience.

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Heavy metal agricultural soil pollution and soil organic matter study, via X-ray fluorescence spectrometry and thermal analysis, in Košice, Slovakia

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Keywords: soil organic matter, TG/DTG/DTA coupled with MS, heavy metal contamination, agricultural soils

In recent years, soil quality and sustainable soils have become increasingly recognized as key factors for the long-term development of society. A wide range of scientific publications are now focused on a better understanding of soils, which is needed to mitigate climate change and ensure long-term economic well-being. For this reason, we focused on monitoring selected agricultural soils from Košice city, that had not been monitored in terms of heavy metal contamination and also of soil organic matter (SOM) and soil organic carbon (SOC) content. As usfull techniques for monitor heavy metal pollution and also SOM, SOC which are one of the soil health indicators we chosen thermal analysis coupled with mass spectrometry and X-ray fluorescence spectrometry. These techniques were chosen, from the point of view, that they are relatively cheap, require a small amount of sample, are fast, and provide reproducible results, that are strongly correlated with a number of basic soil methodologies. Through them we can characterize the complete soil continuum. The studied samples were agricultural soils taken from A horizont from nine different localities in Košice city, Slovakia, which should be contaminated mainly by the influence from industrial discharge. It was found that all studied soils were predominantly strongly alkaline, which should be caused by higher carbonate contents, which was in some cases confirmed via thermal analysis. DTG curves of studied samples show several peaks which means that the SOM have differnet thermal sensitivities which depending on the SOM chemical composition, presence of aliphatic and aromatic structure. Thermal analysis coupled with mass spectrometry provided comparable results to other techniques such as loss of ignition (LOI) in determining the quantity of soil organic matter which was in the range 2.15-4.17%. The maximum content of Zn, Cr, Co, Ni, Cu, Zn, As, Hg and Pb, recorded in topsoils, were as follows: 149.00; 95.50; 23.40; 62.40; 147.00; 149.00; 36.80; 3.7; 40.10 mg.kg^{-1}. These amounts exceeded acceptable levels defined by Slovak law as limited value (LV), especially 1.5-2 times for Co, Ni, Hg, Pb, and according to Europan average value (EAV) 0.5-2 times twice for Ni, Zn, As and Pb. The contamination comes largely from the surrounding industrial processes, such as non-ferrous mettalurgy, iron mettalurgy, vehicular pollution, coal combustion and fertilizers.

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Determination of the temperature and gelation rate of hydrocolloids extracted from fruit pomace by differential scanning calorimetry

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Keywords: DSC, hydrocolloids, fruit pomace

The largest stream of food waste concerns fruit and vegetable raw materials. This is due to improper and/or limited infrastructure, including: improper storage, transport, packaging losses, employee negligence, technical failures, but also waste generated during raw material control and pre-processing. In numbers: 39% of waste is post-production waste, 5% retail and wholesale, 42% is generated by households and 14% by catering services. Food waste has a negative impact on the environment, causing approx. 10% of global greenhouse gas emissions [1]. This problem also concerns insufficient management of biomass generated from food waste. The solution to this problem must be focused on the principles of food waste valorization, reducing the burden on the environment and striving for a closed loop in the food economy [1,2]. The management of fruit and vegetable waste, e.g. for the isolation and production of plant hydrocolloids, allows the use and valorization of part of the waste raw materials.

Hydrocolloids from fruit pomace were obtained using various extraction techniques, e.g. using ultrasound. The gelation parameters of hydrogels in the developed hydrocolloids were determined using differential scanning calorimetry (DSC).

The study showed that hydrocolloids can be obtained from fruit pomace from the fruit and vegetable industry, especially from juice presses. The use of fruit pomace from juice presses allows for the management and reduction of landfill waste. Additionally, the designed hydrocolloids can be used for 3D printing, pharmaceuticals and functional food design. This work was financially supported by the Faculty of Biotechnology and Food Sciences, Lodz University of Technology within the framework of the “COOPERATION” program (project No W5/COOP/03/2024)

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Soil microbial metabolism from a calorimetric and respirometric perspective

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Keywords: microcalorimetry, soil, respirometry, microbial activity

Soil microorganisms are the key players in soil quality, proper functions and fertility. The balance in the soil ecosystem has a broad spectrum of environmental links which are constantly changing. The quality of soil itself clearly depends on the soil organic matter (SOM) content. This is studied by different methods as well as by calorimetry. Isothermal microcalorimetry (TAM III, TA Instruments) can be successfully used to detect microbial life in soil, allowing the exothermic manifestations of the microflora to be monitored. Many factors influence the measurement results: soil freshness (storage time and temperature), moisture, nutrient addition and temperature. In our study, we focused on freshly sampled soil with the addition of different nutrients. The effect of temperature at a set isothermal regime was also monitored. Briefly, the evidence of the presence of SOM in the sample is the exothermic peak caused by the metabolic heat of the microorganisms and the total heat production can be calculated. Heat production was monitored even though the measuring ampoules with the weighted amount of soil were hermetically sealed, and the microorganisms thus had a limited volume of oxygen for their activity. Moreover, the respirometry of the soil samples (carbon dioxide production) was determined using OxiTop® IDS.

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Pet materials for mid-ir reflective properties

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Keywords: heat transfer, human body radiation, IR responsive textile, textile photonic structures, radiative heating, membrane

Space heating is one of the largest energy end-use of buildings. The heating, ventilation and air conditioning system are warming up or cooling down empty volumes. For example, 40% of annual consumption in Europe corresponds to indoor usage, an essential part of which is related to HVAC systems[1]. The ANR project POCOMA aims to reduce building's heating requirements by increasing the thermal efficiency of clothes. Therefore, decreasing the comfort temperature set point in indoor area. Humans lose heat in four ways, i.e., (i) radiation, (ii) convection, (iii) evaporation, and (iv) conduction. It corresponds respectively approximately to 50-60, 20, 15, and 3% of the total body heat loss [2–4]. Reducing indoor temperature without reducing human's mobility, would have a positive impact on the global carbon dioxide emission [1].

Different materials are studied; a white Polyethylene Terephtalate (PET) woven fabric; a spin coated PET membrane structured in photonic crystal (periodic array of hole, diameter 9µm, periodicity 12µm); a spin coated PET membrane on the PET fabric, a spin coated PET membrane glued on the PET fabric and an electrospinned PET nonwoven. The characteristic size of the PET fibres is around 30 µm, and 600 nm for the woven and nonwoven respectively.

An integrating sphere spectrometer will be used to measure the reflectivity in the [8-14 µm] range. Through simulation [5], a 5.8% average reflexion of the non-structured spin coated layer was evaluated. The average reflexion increases to 15.8% thanks to structuration in photonic crystal. Spin-coated layers (structured and non-structured) are under characterization at the moment, to confirm the obtained simulated values.

Thermal characterization, during which samples are placed on a skin model and the temperatures above and below the textile fabric are determined with thermocouples, will soon be carried out.

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Thermogravimetric analysis for assessing changes in soil organic matter pools during amendment-assisted remediation

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Keywords: soil, organic matter, remediation, amendments

The application of organic amendments is a common practice for remediating contaminated soils [1]. Beyond their remediation effects, these amendments also enhance soil organic matter content [2]. However, little is known about whether this increase affects different organic matter pools. Knowledge of changes in soil organic matter stability is essential for assessing its quality and understanding its impact on soil remediation and health [3]. This study aims to investigate changes in labile and recalcitrant organic matter content in soil using a thermogravimetric analyser. A heavy metal-contaminated soil representative of the acidic soils of the tropics—characterized by low organic matter content—was used. The soil was amended with various organic materials, including biochar, poultry manure, and compost. After the incubation period, soil samples were collected for thermogravimetric analysis (TGA) to assess labile and recalcitrant organic matter content. These values were determined from the TGA results. The first signal, observed between 200°C and 400°C, with a peak intensity at 293°C, corresponds to the labile organic matter. The second signal, ranging from 400°C to 600°C, with a peak intensity at 510°C, is associated with recalcitrant organic matter. Additionally, total organic matter content in these samples was determined using the Walkley and Black method. The results indicated that soils amended with biochar had a higher recalcitrant organic matter content compared to those treated with other amendments, particularly poultry manure. In addition to its effects on organic matter, biochar application improved other physicochemical properties, such as pH and cation exchange capacity. In summary, TGA revealed shifts in the distribution of organic matter pools in the soil, providing insight into the impact of amendments on labile and recalcitrant organic matter content. Identifying these changes enables a more informed selection of amendments for large-scale soil remediation and a better understanding of their effects on soil health.

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Determination of the thermal oxidation properties of edible oils commercialized in ecuador by Differential Scanning Calorimetry

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Keywords: Differential Scanning Calorimetry, vegetable oils, crystallization point, melting point, kinetic analysis, fatty acid

Ecuador has a great variety of commercial edible oils that could be obtained from: palm (elaeis oleifera), olive (olea europaea), sunflower (helianthus annuus), corn (zea mays), sesame (sesamum indicum), chia (salvia hispanica), avocado (persea americana), sacha inchi (plukenetia volubilis), among others. Considering that the composition of oils significantly impacts their shelf life, which in turn affects consumer sensory perception and purchasing decisions, it is necessary to fully understand which quality characteristics of oils are derived from the composition of fatty acids. According to this explanation, quality technicians must know how to relate this composition to physical and chemical properties. ATR-FTIR is used to detect changes in oil purity since the -OH functional groups in organic molecules indicate multiple hydroperoxide formations due to the oxidation reaction within the oil samples.

Another suitable method for evaluating these properties is thermal analysis, specifically, Differential Scanning Calorimetry (DSC) is a powerful analytical technique used to assess the thermal properties of oils and fats, providing insights into their oxidative stability, crystallization, and melting points. This method is crucial for predicting undesirable quality characteristics in oils, such as degradation during heating or storage. The thermal oxidation properties were assessed using Differential Scanning Calorimetry in a NETZCH equipment at heating rates of 5, 10, 15, and 20 °C/min. Analyses were performed over two temperature ranges (50 to 300 °C and 50 to –100 °C) under oxidative (air) and inert (nitrogen) atmospheres. The study evaluated thermal decomposition transitions, crystallization and melting behavior, and calculated activation energy using logarithmic kinetic models (Kissinger and Ozawa–Flynn–Wall). The goodness of fit was verified through the Pearson correlation coefficient (R^2).

Among the samples, palm oil showed the highest crystallization temperature (–3.70 °C), while avocado oil exhibited the highest oxidation onset temperatures at all heating rates. Olive oil presented the highest activation energy (Kissinger = 76.395 kJ/mol; FWO = 80.059 kJ/mol), followed closely by sunflower and corn oils, confirming its superior oxidative stability.

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Construction of self-reinforced networks with high-crystallinity silk nanofibrils for ultrafine and biodegradable recycled regenerated silk fibroin monofilament sutures

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Keywords: silk fibroin nanofibrils, self-reinforced network, monofilament sutures

Superfine recycled regenerated silk fibroin (RRSF) monofilament sutures are designed to minimize surgical incisions, prevent scar formation, and facilitate precise suturing in cosmetic and plastic surgeries [1]. However, balancing fineness and strength remains a challenge because the RRSF extraction process disrupts the hierarchical structure of natural silk fibers, leading to suboptimal mechanical properties. This study employed mechanical peeling and grinding to exfoliate β-sheets-rich silk fibroin nanofibrils (SFNF), which served as homologous reinforcing materials uniformly dispersed in the RRSF spinning system [2]. Water-soluble, biocompatible polyvinyl alcohol (PVA) was introduced to enhance ductility. The SFNF/RRSF/PVA (SRP) fiber underwent extensive water immersion stretching to produce ultrafine fibers and foster a highly oriented internal self-reinforcing SFNF network structure. Monofilament surgical sutures were successfully fabricated following surface coating with chitosan. **As shown in Fig. 1**, with 0.1 wt% SFNF (SRP-0.1) and a stretching multiplier of 2.5, the tensile strength of the fibers increased by 33% compared to those without SFNF (SRP-0.0). Fluorescence staining confirmed the presence of highly oriented SFNF networks within the fibers. Mechanical simulations validated the pronounced reinforcement effect of this network structure. The sutures, measuring 39.38 μm in diameter and exhibiting a tensile strength of 0.31 N, met USP standards for 9-0 surgical sutures, making them suitable for microsurgery. Additionally, they demonstrated antibacterial properties, biocompatibility, and degraded at a rate of 43.09% within 30 days. In animal trials, the sutures facilitated wound closure, reduced inflammatory responses, and minimized scar formation.

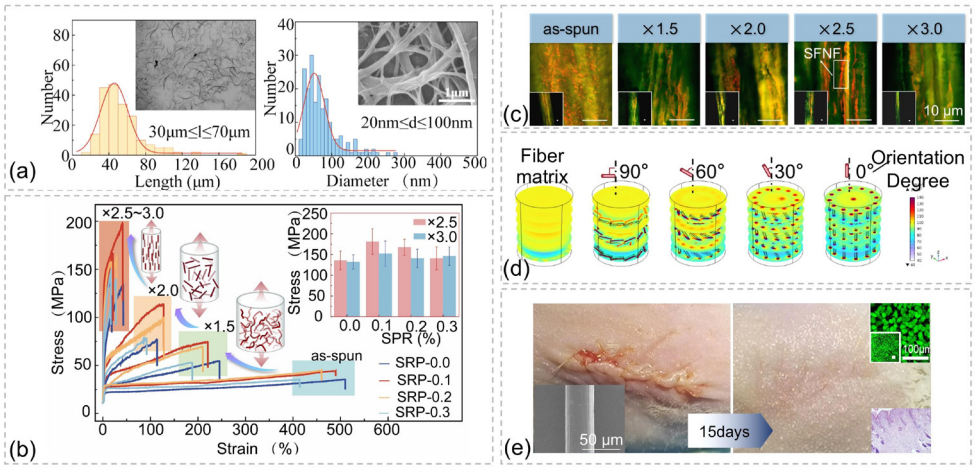

Fig. 1. Frequency distribution of SFNF length and diameter(a), and effect of water immersion stretching on the mechanical properties of SRP fibers (b), dispersion of SFNF in SRP fibers under different water immersion stretching conditions (green fluorescence representing RRSF while red fluorescence representing SFNF)(c), and mechanical simulation results of orientation degree on the mechanical enhancement of SFNF-reinforced networks (d), and the feasibility of the application of surgical sutures (e).

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Physicochemical and antioxidant characterisation of a food supplement based on ginger *(Zingiber officinale),* in vitro evaluation

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Keywords: food supplement, spectroscopic and thermal analysis, ginger

In recent times, there has been a significant rise in the amount of research focusing on natural products due to their outstanding biological properties and positive effects on health. Their pharmacological attributes have played an immense role in detecting natural and safe alternative therapeutics. In this line, ginger *(Zingiber officinale)* has been gaining wide attention owing to its bioactive compounds, such as phenolic and terpene compounds. Ginger has a great pharmacological and biological potential in the prevention and treatment of various diseases, namely colds, nausea, arthritis, migraines and hypertension [1]. The bioactive compounds are unstable and prone to degradation, volatilization, and oxidation when being extracted and processed. This is mainly due to their exposure to environments with adverse conditions, such as high temperature, the presence of O_2 and light.

The purpose of this work is to encapsulate ginger in maltodextrin and add kaolinite in order to amplify the therapeutic effects. The obtained products are characterized by spectroscopy and microscopic techniques (FTIR, RAMAN, SEM). Also, the thermal behavior is studied in the temperature range 25-400°C in the oxidative atmosphere (figure 1) [2-3].

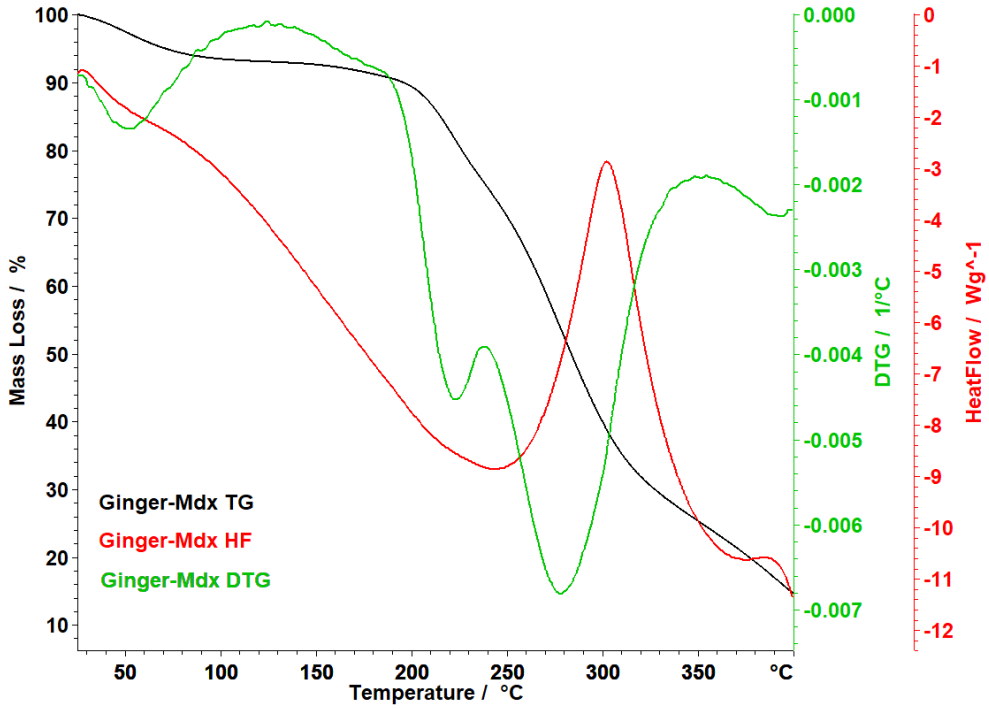

Figure 1. Thermoanalytical curves of Ginger-Mdx

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T02: Calorimetry

Thermodynamic stability and yield of phycolbiliprotein complex of Spirulina platensis after exposure to low (-196^{0}C, -80^{0}C, -40^{0}C, and -20^{0}C) temperatures

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Keywords: Spirulina platensis, phycobiliprotein complex, differential scanning calorimetry (DSC), C-phycocyan.

The study was conducted using the new generation of differential scanning calorimetry (DSC)[1].

The suspension and wet mass of Spirulina platensis was incubated in Zarrouk's medium, pH 10.5, at different temperatures: for 48 hours at -196°C, -80°C, -40°C, and -20°C.

It has been shown that in case of freezing was observed a partial unfolding of biomass including phycobiliprotein complex (PBPc). Calculation of areas under the deconvoluted Gaussian components of DSC curves of Spirulina platensis suspension and wet mass[2] showed that the most perspective approach to receive higher yield of intact PBPc is freezing of the wet mass to -196°C when the sedimentation ratio W/V is 1.5. In this case, the C-phycocyanin (C-PC) and C-allophycocyanin (C-APC) structures are slightly denatured after the cell destruction; 30.79% part of them is totally unfolded, 30.91% is partially unfolded, and 34.3% is not unfolded and remained in their native states.

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Preparation of activated carbons from cd´s waste for SO_2 and NO_x adsorption: a study using adsorption calorimetry

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Keywords: activated carbon, CDs waste, SO_2 adsorption, NO_x adsorption, adsorption calorimetry

Plastic waste, such as CDs, poses an environmental challenge. This study converts CDs into activated carbons using KOH and H_3PO_4, creating microporous structures (1,200 m^2/g, 2 nm pores). Functionalization with amines and acids enhanced adsorption of SO_2 and NO_x, with amino-functionalized carbons showing superior performance due to specific chemical interactions. Characterization revealed surface areas of up to 1,200 m^2/g and 2 nm micropores. Amine-functionalized carbons showed superior adsorption capacities, reaching 75 mg/g for SO_2 and 62 mg/g for NO_x, compared to 45 mg/g and 38 mg/g for non-functionalized carbons. Isotherm modeling indicated that the Sips model provided the best fit for the experimental data, with determination coefficients (R^2) exceeding 0.98 in all cases, suggesting that adsorption processes involved both monolayer adsorption and surface heterogeneity[1,2]. The Freundlich model offered an adequate fit for less-functionalized materials, whereas the Langmuir model was more suitable for systems with highly uniform surfaces. Adsorption kinetics were analyzed using pseudo-first-order (PFO) and pseudo-second-order (PSO) models, with the latter emerging as the most accurate in describing the data, yielding R^2 values above 0.99. The rate constants (k_2) were highest for functionalized materials, reaching 0.035 g/mg·min for SO_2 and 0.028 g/mg·min for NO_x. Finally, adsorption calorimetry was used to evaluate energetic interactions, showing that amine-functionalized materials generated the highest energetic effects, with adsorption enthalpies of up to -120 kJ/mol for SO_2 and -110 kJ/mol for NO_x. These values reflect strong, specific chemical interactions between the gases and the active sites on the carbon surface. In contrast, non-functionalized materials exhibited significantly lower enthalpies (-80 kJ/mol for SO_2 and -75 kJ/mol for NO_x). In conclusion, chemical modifications to the activated carbons substantially enhanced their adsorption capacities and affinities for gaseous pollutants. These results underscore the potential of these materials as sustainable and efficient solutions for capturing gases such as SO_2 and NO_x, contributing to the development of advanced environmental technologies.

Acknowledgments
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Calorimetric analysis of antiferroelectric Pb(Hf1-xSnx)O_3 single crystals (0<x<0.35)

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Keywords: antiferroelectrics, phase transitions, differential scanning calorimetry

Heat capacity of antiferroelectric Pb(Hf1-xSnx)O_3 single crystals (0<x<0.35) was measured in a wide temperature range from 130 K to 730 K by Differential Scanning Calorimetry. The temperatures and orders of particular phase transitions have been determined and the phase diagram obtained was compared to dielectric and structural measurements [1]. The total transition energy and entropy at the phase transitions were calculated. The calorimetric studies for crystals with x<0.08 showed two sharp anomalies typical for first-order phase transitions and associated with phase transitions between two antiferroelectric phases AFE1 and AFE2 and between AFE2 and paraelectric PE phase. Observed anomalies correspond well with the behaviour of the dielectric permittivity as well as the structural data. The thermal hysteresis between heating and cooling process was also observed. The total latent heat and entropy associated with the phase transitions were calculated. The energy transition and entropy changes suggest that the latent heat is mainly governed by the structural changes. As the value of x increases the value of latent heat of all phase transitions decreases. Above the value of x = 0.08 new phase transition has been identified with negligible latent heat confirming the second-order character of this phase transition.

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Thermokinetics – a physicochemical direction in the informatization of concrete technology

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The paper discusses the scientific and methodological aspects of implementing digital technology in concrete production using calorimetric data about the kinetics of exothermic processes in cement and concrete curing. For the first time, foundational physicochemical, technological, and informational principles of concrete science have been articulated.

The thermokinetics framework has been developed to ascertain the directionality, intensity, and completion of curing processes. It demonstrates that both continuous and discrete thermokinetic models effectively quantify the impact of technological factors. The use of thermokinetic analysis in concrete technology has been validated.

A methodology for the discretization of digital calorimetric signals regarding the rate and completeness of processes has been devised. The use of adaptive (self-adjusting) algorithms has proven beneficial for designing concrete mixtures and optimizing curing conditions based on calorimetry data.

The potential of artificial intelligence to forecast thermokinetic curing models for cement and concrete has been explored. The calorimetric approach's prospects in other scientific and technical fields have also been highlighted.

Studying the influence of bone char synthesis settings over its properties and its interaction with glyphosate: application of immersion calorimetry

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Keywords: immersion calorimetry, glyphosate, bone char, enthalpy, surface chemistry

Bone chars with varying properties were produced by altering pyrolysis conditions. In our study, five process variables were evaluated, with the heating rate emerging as the only factor that did not significantly affect the characteristics of the bone char (BC). A suite of analytical techniques—including FT-IR, elemental analysis, gas physisorption, Boehm titration, and pH_{pzc} determination—was employed to elucidate the chemical, structural, and surface modifications that occurred in the bone residues during thermal treatment [1-3].

Statistical analysis indicated that temperature and atmosphere were the two most influential factors governing the properties of BC, affecting its chemical composition, surface chemistry, textural attributes, and microstructure. Notably, the role of nitrogen in the surface chemistry of these materials was identified, with particle size and residence time at peak temperature further modulating this parameter. These findings opened new avenues for investigating nitrogen as a heteroatom within the carbon framework, an aspect that remained underexplored in the literature [4,5].

Furthermore, microcalorimetric techniques revealed that BC exhibited hydrophilic behavior, a characteristic directly linked to its carbon content and, consequently, to the pyrolysis conditions. The interactions between glyphosate and the BC surface were also examined, demonstrating that the surface chemistry of the inorganic matrix (hydroxyapatite, HAP) significantly influenced glyphosate binding. This insight underscored the potential of BC as an effective adsorbent for the removal of glyphosate from polluted water [6].

Acknowledgments
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Optimization of functionalized nanomaterials for gas capture: a study based on adsorption calorimetry

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Keywords: nanomaterials, metal oxides, gas adsorption, adsorption calorimetry, CO_2, NO_x, isotherm models, adsorption kinetics, thermodynamics

The growing concern about emissions of polluting gases, such as CO_2 and NO_x, motivated the synthesis of hybrid nanomaterials based on graphene oxide (GO) and carbon nanotubes (CNT), functionalized with CuO and ZnO nanoparticles and amino groups (NH_2).These materials showed higher adsorption capacities, with maximum values of 45 mg/g for CO_2 on GO-CuO-NH_2 and 50 mg/g for NO_x on CNT-CuO-NH_2, highlighting the synergy between metal oxides and chemical functionalization [1-3].

Characterization by FTIR, XRD, SEM, BET and pH_{pzc} revealed optimal structural and textural properties, while adsorption calorimetry allowed determining negative enthalpies of up to -105 kJ/mol for NO_x, confirming specific chemical interactions. Isothermal models, such as Sips, and kinetic models, such as the pseudo-second-order model, showed excellent fits ($R^2 > 0.98$), evidencing monolayer adsorption mechanisms and surface heterogeneity. The thermodynamic analysis confirmed exothermic and spontaneous processes, with negative $\Delta G°$ (-5.2 kJ/mol at 298 K for CO_2) [4,5].

These results validate the effectiveness of functionalized nanomaterials in capturing polluting gases, underlining the relevance of combining isothermal, kinetic, thermodynamic and calorimetric approaches. This study lays the foundations for developing advanced solutions in environmental mitigation.

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T03: Cements, building materials

Mineralogy of the thermally activated fine fraction of construction and demolition waste

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Keywords: thermal activation, construction and demolition wastes, Differential Thermal Analysis, mineralogical phases

One of the main challenges of present-day society is to reduce CO_2 emissions to the atmosphere as much as possible. A major source of these emissions is produced during the manufacture of cement. The main causes of these emissions are due to the the energy required for the thermal treatment of the raw materials and the CO_2 released during decarbonation. In this study, the thermal activation of fine construction and demolition wastes (CDW) was evaluated for its application as a substitute material for Portland cement in the manufacture of mortars and concretes. The materials investigated consists of fines obtained from the washing of construction and demolition wastes to recover the aggregates. Two types have been differentiated: one contains a fraction primarily composed of concrete (H), while the other is a mixed residue of concrete and ceramic materials (HM). For this purpose, treatments were carried out every 100 ºC between 550 ºC and 950 ºC. Differential thermal and thermogravimetric analyses (DTA-TG) were conducted to determine the optimal temperatures for the thermal treatments. The mineralogy of the phases formed after the thermal activation as well as the amorphous phase content were determined by X-ray diffraction. These data will be highly useful for evaluating the treatment to be applied in its use as substitute materials for Portland cement. To check the reactivity, the R3 test was carried out. The particle size is slightly smaller in the HM wastes compared to the H wastes, with median values of 13 and 22 µm, respectively. The studied CDW show high calcite and quartz contents. Minor phases as clays, feldspars and gypsum occur especially those of mixed components. Minor amounts of ettringite can be present in the H-type wastes and the amorphous phase represents between 25 and 32 mass 5%. The HM waste, has a similar content of amorphous phase. In the residues treated at 650 °C, the components are the same as in the untreated sample, with only ettringite disappearing and a slight increase in the amorphous phase content. At 950 °C, $CaCO_2$ has completely disappeared, and the present mineral phases present are quartz, gehlenite, and larnite, with small amounts of diopside, anhydrite, and hematite. The amorphous phase has been significantly reduced, down to 5% by mass. In the case of slow cooling of the materials, there

are also smaller amounts of lime and pseudowollastonite. The DTA show endothermic peaks corresponding to the dehydroxylation of the hydrated phases (ettringite, C-A-S-H gel, phyllosilicates) and decarbonation of the carbonate minerals. In the H and HM wastes the loss by the decarbonation of calcite and dolomite is 13.6 and 14.5 mass %, which indicates that the carbonate minerals content in the H waste represent 18 % and 30 % of the total mass. These values align with the XRD results. The findings suggest that the CDW will exhibit higher efficiency when treated at 650 °C, and even greater improvement at 950 °C. However, it is important to consider that these thermal treatments require, which may lead to CO_2 emissions. Furthermore, in the case of treatment at the higher temperature, CO_2 emissions will also be produced as a result of decarbonation. Nevertheless, in all cases, these emission values will be lower than those produced during the manufacture of Portland cement.

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Microstructure and phase characterizations of autoclaved high calcium fly ash-calcined clay mortars

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Keywords: microstructure, phase characterizations, thermal analysis, fly ash cements, calcined clay

The use of coal fly ash, a by-product from coal power plant with calcined clay as Portland cement replacement materials was investigated at the total replacement level of 50%. Accelerated autoclaved method was used to produce high calcium fly ash-calcined clay mortars. When autoclaved at 6 and 20 psi, it was found that at 30% fly ash and calcined clay of 20%, the fly ash-calcined clay mix has higher compressive strength when compared to 50% fly ash. Thermogravimetric analysis, scanning electron microscopy and X-ray diffraction were used to determine the phases and it showed that the increased compressive strength of fly ash-calcined clay is contributed to the formation of 1.1nm tobermorite ($C_5S_6H_5$).

Thermogravimetric analysis and phase characterizations of autoclaved fly ash mortars with different calcium oxide content

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Keywords: thermogravimetric analysis, phase characterizations, fly ash, calcium oxide, cements

Fly ash, a by-product from coal power plant, of different calcium oxide content (19% and 28%) were used to replace Portland cement at 50%. The mixes were cured in an autoclave at 20 psi for 6 hours. The results showed that the fly ash with higher CaO content has higher compressive strength when compared to the fly ash with lower CaO content in 50% fly ash mixes. Thermogravimetric analysis (TGA) of the mixes was also carried out to help explain the results by determining the phases in these mixes. X-ray diffraction and scanning electron microscopy were also used.

Use of calcium hydroxide in wood ash-based alkali-activated material

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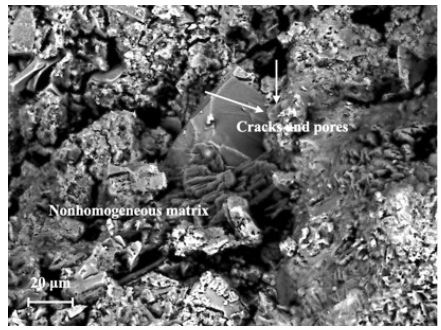
Keywords: waste valorisation, thermal analysis, mechanical properties, mechanism, microstrucure

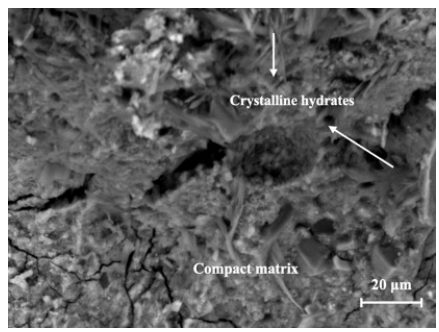
The worldwide concern on sustainable development also proposes demands in the building and construction sectors, focusing on fabricating low-carbon footprint concrete. Alkali-activated materials (AAMs) contribute to less environmental impact, in contrast with the traditional binder material Portland cement, and are regarded as eco-binders. Particularly, the possibility of the incorporation of industrial by-products as precursor materials provides a more sustainable approach for waste management than landfills. Wood ash (WA) is a waste produced in the biofuel energy industry during the procedures of combustion of wood sawdust and chips. With the promotion of renewable clean energy around the globe, the management of WA waste becomes a significant challenge. Unlike other industrial wastes, such as slags and coal fly ash, which have been well researched regarding their application in AAMs, the utilization of WA in building materials is still limited.

In this study, thus, WA, including wood fly ash and wood bottom ash, was used as a precursor to manufacture a waste-based AAM. Recycled sand valorized from biofuel energy plants substituted natural river sand as fine aggregates. Due to the consideration of clean production, as well as to decrease alkali contents in the binder system, calcium hydroxide (CH) was added as a ternary alkaline activator at a ratio of 0, 5, 10, 15, and 20% by precursor mass, besides the conventional activators sodium hydroxide and sodium silicate at a low molarity. To understand the effects of CH content on the engineering properties and microstructure of the produced AAM, a series of tests were conducted, including compressive strength, water absorption, thermogravimetric-differential thermal analysis (TG-DTA), exothermic profiles, scanning electron microscopy (SEM), and X-ray diffraction analysis (XRD).

The results show that the use of CH as a ternary activator greatly contributes to the improvement of the compressive strength within a range between 16.64% and 24.26%. The use of CH powder led to the densification of the AAM microstructure and was related to a reduction of water absorption. In the SEM graphs in Fig.1, the reference sample with 0% CH exhibited a mal-bond microstructure. With a 10% CH addition, a denser morphology was observed. The following increment of CH content to 20% led to less densification of the microstructure. This corresponds well to the strength development. Based on the thermal analysis, CH exerted a positive influence on the facilitation of the early hydration degree, with higher exothermic heat observed during 24 hrs. The TG-DTA examination on the 28-day sample also suggested an increment in the production of hydrates. This was also confirmed by the XRD analysis, where both crystalline and amorphous hydrates were identified.



(a) With 0% CH.



(b) With 10% CH

(c) With 20% CH.

Fig. 1 Micrographs of AAM samples

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Effect of superplasticisers and multiwalled carbon nanotubes on the fresh and hardened properties of cement paste

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Keywords: lignosulphonates, polycarboxylate ether, nano additive, hydration, mechanical properties

Multi-walled carbon Nanotubes (MWCNTs) have attracted significant attention due to their remarkable possibility to improve structure densification and mechanical properties of cement paste. The incorporation of MWCNTs dispersed in carboxyl-methylcellulose can significantly improve the properties of cement paste. However, the behaviour of cement paste is significantly influenced by the incorporated amount of MWCNTs and the type of superplasticiser used. In this study, two types of superplasticisers, lignosulphonates (L) and polycarboxylate ether (CE), were employed as dispersing agents for MWCNTs to improve the interfacial affinity between MWCNTs filaments and cement and to enhance the strength of the cement paste. For this reason, MWCNTs ultrasonication together with SPs was conducted. This work used microcalorimetry, conductometry, pH, and setting time to evaluate cement hydration properties. SEM, XRD, and DTA/ TG tests were used to evaluate the structure of the hardened cement paste. Experiment results revealed that using a higher amount of MWCNTs effectively facilitates the hydration process of cement at the early stage of hydration. However, in the presence of SP(CE), the hydration process and setting time of cement are noticeably prolonged due to lower pH values in the paste. On the contrary, the interaction of CNTs with SP(L) quickens the hydration process due to additional ettringite creation. XRD and DTA/TG studies confirmed that a higher amount of ettringite is detected in cement pastes incorporated in MWCNTs and SP(L). However, the higher amount of portlandite and CH formed is responsible for the better mechanical properties of the SP(CE) cement paste samples.

Valorization of concrete washing slurries for environmentally friendly applications

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Keywords: construction and demolition waste fines, thermal analysis, waste reuse, circular economy

The fine fraction of construction and demolition wastes is widely investigated as possible substitute for Portland cement in concrete manufacturing. Some concrete manufacturing plants receive waste from the washing of concrete mixers and product that were not delivered on time. The aggregates from these concretes are washed and reused in the manufacture of new concrete mixtures. However, fine particles are typically not recycled and are instead sent to landfills. This study investigates the feasibility of a new utilization of fine particles from fresh mortar and concrete at a concrete plant from Catalonia. It has been characterized in order to assess its applicability as a substitute for Portland cement in the production of mortar and concrete. Also, some tests have been conducted to verify the effectiveness of these wastes as neutralizers of acidic waters and compared with experiments using limestone powder. Both materials were always used with a similar particle size, averaging approximately 12 μm. For these purposes, the chemical composition has been determined using X-ray fluorescence, the mineralogical characterization was studied using X-ray Diffraction (XRD), Fourier Transform Infrared Spectroscopy and Scanning Electron Microscopy (SEM), and the thermal properties were analysed using Differential Thermal and Thermogravimetric Analysis (DTA-TG). Their chemical composition is similar to that of Portland cement, with a slightly lower CaO content, 49-51 mass%. Regarding the crystalline phases, these residues mainly contain quartz, calcite and portlandite along with smaller amounts of ettringite, dolomite and phyllosilicates. The proportion of the amorphous phase was determined by introducing a known percentage of corundum, revealing that it is present in a significant amount. This is the C-S-H gel phase produvcen during the hydration of cement, which has also been observed in the SEM. Regarding their thermal behaviour, the DTA-TG shows the presence of three endothermic peaks. The first occurs around 125 °C and is attributed to the dehydroxylation of ettringite and the gel phase. The second takes place at 500 °C and is caused by the loss of OH^- from portlandite, and the third, at 867 °C, is due to the decarbonation of calcite and dolomite. The mass losses associated with these events were 13%, 4%, and 17.5%, indicating the presence of 12 mass% portlandite and 40 mass% calcite in the waste. The results demonstrate that these residues are suitable for several potential applications. One of them is the use as substitute to Portland cement in the production of mortars and concrete. To enhance the binding properties these materials should be thermally activated at the decomposition temperature of portlandite, slightly higher than 500 °C. The properties are improved at 900 °C, however, it should be considered that in this case, calcite is transformed into CaO and CO_2. Additionally,

they could serve as an effective neutralizer for acidic waters. The tests carried out showed higher efficiency of these wastes than the limestone powder. This was to be expected, due to the greater effectiveness of portlandite and the gel as agents for neutralizing acidity.

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Resistance of LC^3 cement pastes against supercritical CO_2 attack

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Keywords: LC^3 pastes, calcined clay, limestone, silica fume, metakaolin, supercritical CO_2

Limestone calcined clay cement (LC^3) is a promising alternative to traditional cementitious materials. Main admixtures of this concept, clays and limestone, are widely available materials all over the world, making it a practical and sustainable choice for producing low-carbon cement. Previous results have shown that even with a 50 mass % replacement of cement by admixtures, mechanical properties comparable to plain Portland cement are achieved [1]. Besides, good resistance in presence of sulphates and chlorides has been proven [2,3].

Based on ongoing research into the use of LC^3 in various environments and the promising results demonstrated to date, we decided to investigate utilization of LC^3 in the cementing of geothermal wells with particular emphasis on resistance against supercritical CO_2 ($scCO_2$).

Studied LC^3 samples consisted of clinker up to 50 mass %, calcined clay and limestone in a ratio of 2:1, and gypsum. Reference cement paste was prepared only from Portland cement. Samples from conventional cementitious materials were examined for comparison. Silica fume and metakaolin used as admixtures accounted for 30 mas % of the mixture. Water to binder ratio was 0.44. Except for the reference cement paste, a superplasticizer was added to improve the rheology of the samples. After 24 hours, the samples were demoulded and placed in a high-pressure vessel. Supercritical CO_2 conditions were achieved by gradually pressurizing with CO_2 up to 10 MPa and heating to 70 °C. The samples were exposed to these conditions for 7 days. All studied compositions were also subjected to standard water curing for 7 days to evaluate the effect of $scCO_2$. The samples were assessed by means of TGA, XRD, FTIR, SEM, and compressive strength measurements.

Based on the results, the carbonation depth of LC^3 was higher than that of reference mix and mixes from conventional cementitious materials and increased with increasing clinker substitution. Higher carbonation depth in LC^3 could be explained by more porous structure and lower amount of CH depleted in pozzolanic reactions of calcined clay and because of dilution effect. Carbonation of CH results in volumetric expansion and causes densification and reduction of pore volume. Therefore, at lower CH content, the pore structure is more permeable and the CO_2 ingress less constrained.

Besides, lower content of CH led to lower CO_2 adsorption capacity, so even though the CO_2 has penetrated to a greater depth in the case of LC^3 systems, amount of newly formed carbonates was the smallest.

As a result of supercritical CO_2 exposure, the compressive strength of all samples increased compared to the corresponding samples cured in water. An almost twofold increase was observed in the reference cement paste and samples blended with MK and SF, reaching over 80 MPa. The lowest carbonate content in LC^3 systems resulted in a smaller increase in compressive strength.

Acknowledgments
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Influence of fly ash replacement on monoliths subjected to acid and base solution attack

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Keywords: fly ash, cement, acid solution, base solution, monoliths, attack

Fly ash, a residue from waste incineration and coal-fired power plants, poses significant environmental and public health challenges due to its fine particulate nature and potential content of hazardous substances like heavy metals [1-2]. While safe landfill disposal is a common practice, a more beneficial approach involves utilizing fly ash in the cement industry to enhance the chemical and physical properties of cement clinker. Over the past decade, the use of fly ash as a partial cement replacement has gained traction, with studies indicating that incorporating up to 30% fly ash from sources like sugar cane and bituminous coal can maintain the strength of cementitious materials [1-4]. This study investigates the feasibility of using fly ash as a sustainable alternative in construction, capitalizing on its potential environmental advantages and ability to improve concrete properties. Faced with a high demand for concrete and the pressing issue of solid waste management, sustainable alternatives are crucial [3]. This research focuses on analysing the performance of concrete mixtures incorporating sugar cane fly ash, coal fly ash, and crushed green glass as a substitute for conventional concrete aggregates. The experimental program included assessments of compressive strength, pH levels, neutralization depth, and water absorption. Furthermore, thermogravimetric analysis (TGA) was employed to characterize the crystalline phases within the hydrated cementitious materials. Samples for TGA were prepared by extracting representative portions after compressive strength testing, arresting hydration with acetone immersion, and subsequent desiccation. A TGA Discovery 5500 (TA Instruments, Agilent) was used for analysis, with a temperature ramp from 30 °C to 600 °C at a heating rate of 10 °C/min under a nitrogen atmosphere (N2 UAP). The resulting thermogravimetric curves were analysed to identify and quantify crystalline phases formed during cement hydration. Six distinct concrete mixture designs were created, tested, and analysed at specific curing ages. The results indicated that mixtures containing bituminous coal fly ash exhibited the most promising performance. The mixture incorporating crushed green glass showed significantly lower strength, suggesting that further evaluation is needed to determine its viability and potential applications in construction. The concrete samples displayed basic alkalinity and were found to be in a non-carbonated state. Future research should extend this investigation to include the evaluation of structural elements like beams and tanks and consider the addition of corrugated steel reinforcement to assess the composite behaviour and long-term durability. The impact of using fly ash on the ecosystem and human health has been shown to be reduced when utilizing even small percentages of fly ash.

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Evaluation of the deterioration of monolith specimens made of fly ash-cement mixtures subjected to leachate from the doña juana sanitary landfill

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Keywords: fly ash, cement, leachate, deterioration

Fly ash from waste incineration processes is a problem for both the environment and public health. Due to their particle size and the substances, they may contain, such as heavy metals, in many cases they must be disposed of in safe sanitary landfills. In the best of cases, they are used in the cement industry in the cement clinkerization process to improve its chemical and physical properties. In the last decade, the use of this material as a cement substitute has been increasing. Some researchers have found that additions of up to 30% in the case of ash from sugar cane and bituminous coal, can maintain the strength properties of the materials [1-4]. This study investigates the feasibility of incorporating fly ash as a sustainable substitute in construction materials. Fly ash, a byproduct of waste incineration processes, offers potential environmental benefits and can enhance the properties of concrete. Driven by the high global demand for concrete and the escalating challenges of solid waste management, the exploration of sustainable alternatives is paramount. The aim of this research is to analyse the performance of concrete mixtures incorporating sugarcane and bituminous coal fly ash, as well as crushed green glass as a concrete aggregate replacement. The experimental methodology included assessments of compressive strength, pH levels, neutralization depth, and water absorption. Furthermore, the crystalline phases present in the hydrated cementitious materials were characterized using thermogravimetric analysis (TGA). To prepare the samples for TGA, representative portions were extracted following the compressive strength testing. Hydration was immediately arrested by immersing the samples in acetone, and subsequently, the solvent was removed by placing the treated samples in a desiccator. The prepared samples were then analysed using a TGA Discovery 5500 (TA Instruments, Agilent). The analysis was conducted under a nitrogen atmosphere (N_2 UAP) as the purge gas, with a temperature ramp from 30 °C to 600 °C at a heating rate of 10 °C/min. The resulting thermogravimetric curves were then used to identify and quantify the crystalline phases formed during cement hydration. Six distinct concrete mix designs were formulated and tested at specific curing ages to evaluate their performance. The results indicate that concrete mixes containing bituminous coal fly ash exhibited the most promising performance characteristics. Conversely, the mix incorporating crushed green glass demonstrated significantly lower strength compared to the other mixes. This suggests that further investigation is necessary to determine the viability of crushed green glass and to identify potential applications in construction where its properties are suitable. Furthermore, the concrete samples displayed a basic alkaline nature and were found to be in a non-carbonated state at the time of testing. Based on these findings, it is

recommended that future research extend this investigation to include the evaluation of structural elements such as beams and tanks. Additionally, studies should consider the integration of corrugated steel reinforcement to assess the composite behaviour and long-term durability of these alternative concrete mixtures.

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Application of inert mineral fillers for practical ecological solutions in cement mortars

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Keywords: cement mortars, mineral filler, XRD, Scanning electron microscopy, ecology

One of the main approaches to reducing the environmental impacts of the construction industry is the use of mineral additives reducing the use of cement in mortars and concretes for construction [1, 2]. The objects of this research are different cement composites with high content of inert mineral fillers (marble). This work investigates the influence of inert mineral fillers and low water-to-cement ratio on the microstructure and hydration of White Portland cement. The evolution of the curing processes and the crystal formation during up to 120 days of water-curing are also studied. Attention was focused on the general microstructural development during curing and observed calcium silicate hydrates (C–S–H), portlandite and carbonate-containing phases.

The phase composition (newly-formed phases as well as the formation of C–S–H gel) is determined by powder X-Ray diffraction, Physical-mechanical properties, and SEM. The experimental data shows that the cement composites containing inert marble filler as an additive lead to the creation of carbo-sulpho-aluminates. A significant reduction in the workability of the fresh mortars is not observed. Testing of samples with high inert mineral fillers content showed that their structure is denser. Prolonged hardening of the cement systems under constant access to water increases their compressive strength by 17.9%.

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Calcium formate as accelerator of LC^3 cement hydration

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Keywords: LC^3 cement, hydration acceleration, calcium formate, isothermal calorimetry

The concept of "calcined clay limestone cements" (LC^3) is part of broad global initiative focused on reduction of CO_2 emissions related to production of cement and building the concrete structures [1]. Specifically, this approach lies in reduction of Portland clinker content as the most energy and CO_2 intensive component of cement. The mixture of 50% of clinker, 30% of calcined clay, 15% of limestone and 5% of gypsum may be understood as typical example of LC^3 cement. Calcined clay is example of Supplementary Cementing Material (SCM) which is activated in concrete by $Ca(OH)_2$ produced during the C_3S hydration and thus providing additional C-S-H hydration products. The well-known limit of concrete based on blended cements (Portland clinker with a SCM, including LC^3) is the slower hydration (compared to Portland cement) resulting to lower early age strength. This unwanted effect (with respect to the construction works progress) should be overcome either by optimized cement milling procedure, or by acceleration of pozzolanic reaction of calcined clay, or by acceleration of clinker hydration (and consequently the pozzolanic reaction) [3].

One of possible approaches to accelerate the clinker hydration is adding of a soluble salt to the concrete mixture [4]. Among them, calcium salts are the most effective in Portland cement [5]. The mechanism of hydration acceleration by calcium salts is not fully understood, however there is lot of partial processes during the hydration which are influenced by e.g. calcium nitrate [6]. The present research aims to study the effect of calcium formate on the hydration and setting/hardening of LC^3 cement; calcium formate is positively influencing the Portland cement hydration [7]. The hydration course was monitored by isothermal calorimetry, the acclerationg effect was evaluated by setting time and early strength determination. It was found that 2% of calcium formate per clinker dose are effective acceleration additive of LC^3.

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Octane-expanded perlite PCM composites for thermal management in buildings

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Keywords: PCM composites, energy storage, thermal analysis

Perlite is a low cost and abundant volcanic mineral with a high-water content within its structure. When heated this water molecules are used to expand the material. The obtained expanded perlite is chemically neutral, inert to atmospheric agents and the passage of time, non-combustible, non-toxic and insoluble. The expanded perlites high porosity allows its usage as a simple way to macro-encapsulate phase change materials (PCM). As a PCM material we used - Octadecane an alkane hydrocarbon with the chemical formula CH3(CH2)16CH with a melting point in the range of 28-30ºC and a heat capacity of 2.22 J/K·g. We used this organic PCM because is the alkane with the lowest carbon number that is unambiguously solid at room temperature and having the melting point close to the human's comfort zone.

The PCM composite was fabricated using vacuum infiltration (~ 10^{-1} torr at 40ºC) of the melted octadecane into the expanded perlite particles. The obtained composite was coated to seal the pores to improve its long-term stability. The perlite particle size was in the range of 2-4 mm, separated by sieving. The particles porosity was estimated using image analysis on SEM observations. The starting PCM and the manufactured composite was thermally characterized by DTA analysis. The composites stability was evaluated by measuring the weight modification after 10 heating and cooling cycles.

Effect of metakaolin waste as a pozzolanic additive on the hydration processes and properties of cement stone

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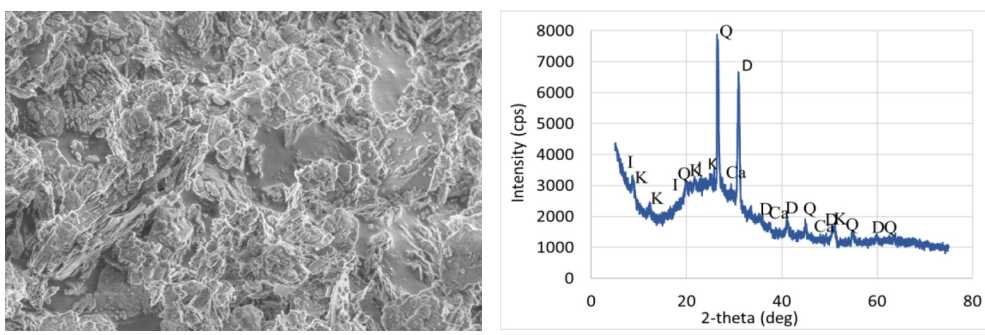
Keywords: hydration heat, cement stone, metakaolin waste, pozzolianic additive, properties

The study examines the effect of metakaolin waste, characterized by high pozzolanic activity (1451 mg/g), on the hydration processes of cement paste and the properties of cement stone. Extremely fine (average particle size 4.79 µm), characterized by a large amount of amorphous phase, metakaolin waste SEM and XRD pattern images in Figure 1 are formed at a certain stage of the technological process of foam glass granule production. Since the average particle size of metakaolin is smaller than the particle size of cement, a minimum amount of metakaolin waste (up to 10 %) was used in the studies as a cement substitute. During the study, six batches of samples were produced, in which from 0 % to 10 % of cement was replaced with metakaolin waste. After evaluating the physical and mechanical properties of cement stone, it was found that replacing 8 % of cement with metakaolin waste results in cement stone with up to 30 % higher strength and denser structure.

The release of heat of hydration and the formation of phases are temperature-sensitive processes [1]. The use of metakaolin waste leads to a rapid initial heat release, followed by a decrease in the heat release rate [2]. In addition, waste such as metakaolin can be used as a cement substitute [3], reducing the overall environmental impact of production.



a) b)

Figure 1 a) Microstructure images of the metakaolin waste; b) XRD analysis results of metakaolin: Q – quartz; D – dolomite; K – kaolinite; I – illite; Ca – calcite.

In all samples, a temperature peak of the exothermic reaction is observed after 6-8 hours [4]. By increasing the amount of metakaolin replaced into cement to 10 % in the composition, the temperature of the exothermic maximum reaction decreases by 8.8 %. Metakaolin waste, due to its fineness of particles and the formation of hydration products, increases the density, strength, water resistance of concrete, and improves the durability of cement stone.

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Develop a new instrument to test the bond strength of reinforced concrete at high temperatures

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Keywords: bond strength, reinforcement concrete, pull-out test, high temperature, instrument design

In order to understand the impact of high temperatures on the bond strength between steel bars and concrete, this study referred to the research [1-3] to design an instrument that can conduct steel bar pull-out tests at high temperatures, as shown in Figure 1. Its heating temperature can reach a maximum of 1000°C. A thickened, strong steel plate is installed inside the instrument to support the specimen's tensile stress during the steel bar pull-out test. In addition, a reinforced frame is made to fix the instrument during the test, prevent it from moving during the pull-out test, and protect the instrument door from being bounced open when the concrete is explosive due to high temperature, endangering operators. The test results show that the concrete with blast furnace slag (replaced 60% weight of cement) was subjected to high-temperature up to 800°C and then kept for 1 hour; a pull-out test of the steel bar was conducted. Its bond strength was 6.8 MPa, lower than the 7-day bond strength of pure cement concrete without subjecting it to elevated temperature. The concrete presented an earthy yellow color with many hair-like cracks on the surface. In addition, the concrete exploded at around 300°C. Because the concrete incorporates 0.15% steel fiber and polypropylene fiber, the explosive phenomenon of concrete is not severe; only spalling occurs on the surface of the concrete (Figure 2). Another concrete specimen was elevated to a high temperature of up to 400°C, kept for 1 hour, and conducted pull-out test. Its bond strength of 10.7MPa was higher. The concrete appeared gray, with obvious splitting cracks and no spalling.

Figure 1 Test instrument.

Figure 2 High-temperature spall of concrete.

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T04: Ceramics, glasses

Vitrification of contaminated technosoils as a remediation strategy with economic benefits

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Keywords: vitrification, industrial soil, differential thermal analysis, viscosity evolution

Vitrification is a promising methodology to stabilize different types of waste, including urban residues, tailings, and technosoils. This process is particularly effective because glass, with its durable structure, can trap hazardous pollutants and heavy metals. Contaminated soils, especially those with heavy metals, can have application in industry to produce glasses and glass-ceramics. The aim of this study was to assess the viability of ex-situ vitrification as remediation strategy for an Hyperurbic Technosol (Loamic, Calcaric, Eutric) from the former industrial neighbourhood of El Clot in Barcelona, Spain. Five batch compositions were prepared using these soils and different alkali additions to enhance the fluidity of the glasses, and Sb to promote glass discoloration. The final glasses compositions plot within the glass-forming region of the SiO_2-CaO-Al_2O_3 system. The vitrification was carried out with a treatment at 1300-1450 ºC and a holding time of 2 hours. Energy costs are similar to those used to produce soda-lime-based commercial glass. X-ray fluorescence (XRF), X-ray diffraction (XRD), dilatometry and hot stage microscopy (HSM) colorimetric spectroscopy were used to characterise the soil and the obtained glass. Differential thermal analysis and thermogravimetry (DTA-TG) was used to obtain the nucleation and crystallization temperatures to be applied to manufacture a glass-ceramic. The efficiency of the method for sequestering hazardous cations were analysed by inductively coupled plasma-optical emission spectroscopy (ICP-OES) following the DIN 38 414 S4 standard. The main components of the soil are SiO_2, 58.9 wt.%; Al_2O_3, 12.6 wt.%; TiO_2, 0.7 wt.%; Fe_2O_3, 4.8 wt.%; Na_2O, 0.7 wt. %, CaO, 6.6 wt.%; MgO, 1.4 wt.% K_2O, 2.50 wt.%: MnO 0.1 wt.% and P_2O_5, 0.3 wt.%. The main potentially toxic elements are As 19 $mg \cdot kg^{-1}$; Cr 129 $mg \cdot kg^{-1}$; Cu 78 $mg \cdot kg^{-1}$; Hg 29 $mg \cdot kg^{-1}$; Ni 28 $mg \cdot kg^{-1}$; Pb 154 $mg \cdot kg^{-1}$ and Zn 257 $mg \cdot kg^{-1}$. The mineral composition of soil is 29 wt.% quartz, 41 wt.% illite, 4 wt.% chlorite, 5 wt.% K-feldspar, 18 wt.% plagioclase, and 4 wt.% calcite. The transition and dilatometric temperatures (T_g and T_d) of glasses were determined by dilatometry, obtaining T_g values of 544 to 576 ºC and T_d 619-636 ºC. The Tg values obtained by dilatometry or DTA have a variation around 45ºC. According the difference between the viscosity temperatures 10^6 and 10^3 Pa-s, the workability range of the glasses produced can be classified short because their ranges are between 264-269 ºC ($\Delta T <$ 400ºC). The temperatures for the viscosity fixed points were measured by HSM; first shrink-

age at $10^{7.9}$ Pa s occurs at 725-782 ºC; maximum shrinkage at $10^{6.9}$ Pa s occurs at 819-881 ºC, softening at $10^{5.6}$ Pa s is at 894-926 ºC; half ball at $10^{3.5}$ Pa s is at 1127-1156 ºC and flow at $10^{2.1}$ Pa s is at 1200-1269 ºC. The glass leaching results show a good retention of As , Cr, Cu, Hg , Pb , Ni and Zn. It can be concluded that vitrification represents a good proposal for the remediation and valorisation of contaminated soils.

Viscosity of model barium crystal glasses

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Keywords: barium crystal glass, viscosity, fragility, Q-units, activation energy

The temperature dependence of viscosity of model barium crystal glasses was studied. The composition of fifteen studied glasses was derived from the composition of currently produced (RONA, a.s. Lednické Rovne) barium crystal glass (10.49 mol.% Na_2O·2.36 mol.% K_2O·9.06 mol.% CaO·0.78 mol.% ZnO·2.44 mol.% BaO·0.85 mol.% Al_2O_3·74.02 mol.% SiO_2) by increasing/decreasing the content of each particular oxide and retaining the same relative amounts of the other oxides. The composition of the prepared glasses was determined by X-ray fluorescence spectrometry (XRF). Due to uncontrolled volatility of alkali oxides the composition does not fulfil the prescribed pseudo-binary character for samples with changed amount of particular oxide. The temperature dependence of viscosity was measured by thermomechanical analysis (high viscosity / low temperature) and rotational viscometry (low viscosity / high temperature). The Vogel Fulcher Tammann equation (VFT) was used for description of viscosity temperature dependence. The glass transition temperature (log $\eta(T_g)$/dPa.s = 13) and fragility (m) were evaluated from VFT parameters. The activation energy of viscous flow (E_{akt}) was evaluated from the low temperature viscosity described by the Andrade`s equation. The Shakhmatkin Vedishcheva thermodynamic model (SVTDM) was evaluated for each glass composition. From 58 considered components of SVTDM only 25 with non-negligible equilibrium amount were found. From SVTDM the Q-units distribution was evaluated. By multilinear regression analysis the dependence of considered quantities (T_g, E_{akt}, m) on molar amounts of various Q-units was evaluated. The obtained results confirmed that the viscosity behaviour of model barium crystal glass can be described by Q-distribution with sufficient accuracy.

Tab. 1. Activation energy, glass transition temperature, and fragility of studied glasses.

glass	FUT	Si+	Si-	Na+	Na-	K+	K-	Ca+	Ca-	Al+	Al-	Ba+	Ba-	Zn+	Zn-
E_{akt} [kJ.mol-1]	459	407	538	508	483	476	510	529	426	477	462	467	488	481	479
T_g [°C]	524	533	519	501	557	517	531	501	539	527	518	522	529	522	525
m_{VFT}	40	36	50	44	40	42	41	45	38	40	40	41	39	43	43

Acknowledgments
This work was supported by The Slovak Grant Agency for Science under grant No. VEGA/1/0021/23, 2/0043/25, and by the Research and Development Support Agency APVV-21-0016 and APVV-22-0004.

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Thermo-mechanical and corrosion study of barium crystal glasses

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Keywords: barium crystal glass, glass transition, corrosion, roughness

The 15 glass-forming melts with the composition derived from the barium crystal glass (10.49 Na2O·2.36 K2O·9.06 CaO·0.78 ZnO·2.44 BaO·0.85 Al2O3·74.02 SiO2) by increasing/decreasing the content of each oxide was measured by thermo-mechanical and corrosion properties. The amorphous character of the prepared glasses was demonstrated via X-ray diffraction (XRD) analysis. The composition of the prepared glasses was determined by X-ray fluorescence spectrometry (XRF). The glasses were measured thermomechanical analysis. Thermodilatometry was measured vertical TA Q400 EM dilatometers. The highest value of the transformation temperature was obtained for the Na MM sample with a value of 557.1°C and the lowest value was obtained for the CaPP glass with a value of 500.9°C, Fig. 1. The coefficients of thermal expansion for the studied glasses were measured in the temperature range from 307°C to 624°C. The 10 randomly selected places of the sample surface with an area of 1.68 x 1.41 mm were analyzed. The sum of the results of the arithmetic mean height (Sa) for all studied samples. The highest roughness was observed for the sample with a corroded surface of Na PP with a value of 0.95 mm and the lowest was for Si PP with a value of 0.63 mm. From the results, it is possible to observe a demonstrable difference in roughness before and after the corrosion tests.

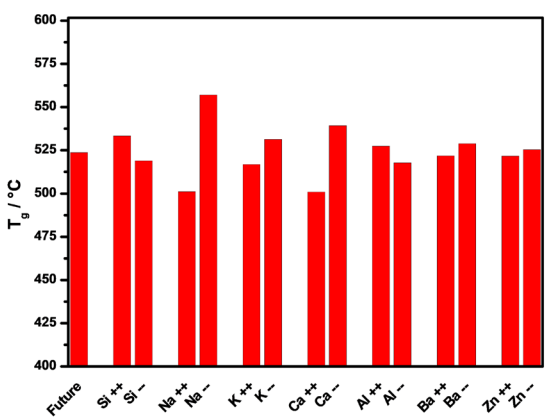

Fig. 1. Comparison of Glass Transition Temperatures (T_g).

Acknowledgments

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Evaluation of the properties of silica materials dotted with silver nanoparticles

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Keywords: silica nanospheres, silver-functionalized nanoparticles, thermal analysis, SEM, antibacterial properties

Silica is a very popular material used in nanotechnology, as an additive to polymers, biomaterial, dental fillings and others. The wide use of silica is related not only to the general availability of this material, but also to its specific properties and possibilities of creating various types of nanostructures, consisting not only of SiO_2, itself, but also as hybrid combinations of SiO_2 with other materials. The most common forms are silica nanoparticles obtained as hybrid spherical particles consisting of a core and a surface nanolayer, called *nanoshells* or *core-shell* [1]. One of the most frequently studied systems are *core-shell* silica nanoparticles, where the silica core is covered with a thin layer of a noble metal, however, an alternative approach was used in this work, consisting in dot deposition of silver on the surface of SiO_2 (so called *dotted silver-silica nanoparticles*). The synthesis of nanospheres was carried out by the Stöber method, using tetraethoxysilane (TEOS), water and ammonia water as a basic catalyst. The process was carried out in ethanol, at a molar ratio of TEOS to water of 0.0047 and in the presence of ammonia water in the range of 0.10–1.25 mol. The obtained silica spheres had a diameter in the range of 50–500 nm, which was confirmed by scanning electron microscopy (SEM) and dynamic light scattering (DLS). Then, through controlled functionalization, silver was dotted on the surface of the spheres, creating nanomaterials with potential antibacterial properties. The characterization of the obtained nanomaterials also included zeta potential measurements to determine colloidal stability, infrared spectral analysis (FTIR) to identify functional groups, and thermal stability assessment using differential scanning calorimetry (DSC) in the temperature range between 20 and 1000°C, coupled with the analysis of gases emitted during heating of the sample. The antibacterial properties of functionalized nanospheres were determined using the Kirby-Bauer disk diffusion method, examining their effectiveness against selected bacterial strains. The results of the study indicate that silver dotted on silica nanospheres allows obtaining a nanomaterial with potential antibacterial properties, which makes possible to use of such materials as a component of protective coatings with antibacterial properties.

Acknowledgments
Research project supported by the “Excellence initiative-research university" program for the AGH University of Krakow.

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Analysis of physicochemical properties of clinker tiles with the addition of alternative waste raw materials

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Keywords: ceramic tiles, thermal analysis, mechanical properties, XRD analysis

Ceramic tiles add aesthetic value to utility surfaces, but above all they are durable materials that do not deteriorate over a long period of use. This applies to both highly sintered tile materials, intended primarily for floors and walls indoor and outdoor, such as porcelain gres, clinker or stoneware materials, but also materials with water absorption above 0.5%, used primarily as wall cladding inside buildings. A very important element that plays a key role in the production of ceramic tiles are the raw materials based mainly on natural raw materials, i.e. clay raw materials, feldspar raw materials and quartz sands. Among the listed raw materials, a special role is played by raw materials contributing to strong sintering, including clay raw materials showing a large sinterability interval in the range of 1100-1200°C and feldspar raw materials (flux raw materials), which contribute to the intensification of sintering processes during firing. In this study, some of the classical raw materials in the raw material composition for clinker ceramic tiles were replaced with an alternative waste raw material (fly ash from waste incineration) and tile compositions were designed, in which the content of the waste raw material varied in the range of 2-8%wt. For the prepared sets of masses, an analysis was carried out of the effect of adding an alternative waste raw material on the physicochemical properties, in particular thermal and mechanical properties of the obtained materials. The prepared masses in the form of granulates with a moisture content of 6% were first tested to determine sinterability using a high-temperature microscope HSM and dilatometric measurements. In the further part of the work, samples were pressed from the prepared granulates and fired in the temperature range from 1120 to 1200°C, for which the phase composition was determined using X-ray analysis (XRD), linear changes in the samples, and measurements of the degree of sintering were performed, determining water absorption, porosity and apparent density in accordance with the PN-EN ISO 10545-3 standard. Mechanical bending strength measurements were also carried out after firing, using the three-point bending method. X-ray analysis of the masses after the firing process showed the same phase composition for the individual masses, regardless of the amount of the alternative raw material introduced. The measurements of water absorption, open porosity and apparent density showed that the introduction of fly ash improved the functional parameters of the products (reduced water absorption and open porosity). The assessment of water absorption and open porosity of the samples showed that with the increase in the share of ash in the masses, the

water absorption and open porosity of the materials decreased. The introduction of fly ash to ceramic masses caused a significant increase in the bending strength of sintered materials, and all tested samples with the addition of ash showed an increase in bending strength compared to the reference sample without the addition of ash. Sinterability measurements using the high-temperature microscope further revealed that the introduction of fly ash lowered both the initial sintering temperature and the temperature at which maximum sintering occurred. It can therefore be stated that the introduction of ashes to ceramic masses allows for the replacement of some natural raw materials, the resources of which are limited, but can also be one of the methods of managing ashes that are waste from the combustion process.

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Thermodynamic model and structural analysis of borosilicate glasses

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Keywords: borosilicate glass, thermodynamic model, Q-distribution, molar volume

A study was focused on 17 samples of borosilicate glasses, utilizing an eight-component model system representing the pharmacy vials with the following base glass composition: 75.23 mol% SiO_2, 7.70 mol% B_2O_3, 4.24 mol% Al_2O_3, 8.02 mol% Na_2O, 1.15 mol% CaO, 1.44 mol% K_2O, 0.95 mol% ZnO, and 1.26 mol% BaO. The glass compositions were modified through increasing and decreasing the molar amount of each oxide. For the network-forming oxides (SiO_2, B_2O_3, and Al_2O_3), the content was changed by ±10 relative %. For the modifier oxides (remaining oxides), the content was either increased by ±40 relative % or reduced to the zero.

Molar Gibbs energies from the FACT database were used to calculate the Shakhmatkin-Vedishcheva thermodynamic model (SVTDM). 115 model components were considered, of which only 25 with non-negligible equilibrium molar amount were identified. After identification of strongly correlated components, only 11 independent components remained.

From the SVTDM results, the distribution of Q_{Si} and Q_B was calculated. Multilinear regression analysis was used to describe the dependence of (V_m) and (T_g) on the abundances of significant and uncorrelated SVTDM components. After excluding statistically insignificant terms for (V_m) and (T_g), s_{apr} of 0.61 cm^3/mol and 18.3 K were obtained. Subsequently, regression analysis was used to describe the dependence of (V_m) and (T_g) on the molar amounts of the individual Q-units. Following the removal of statistically irrelevant terms for (V_m) and (T_g), s_{apr} 0.23 cm^3/mol and 6.2 K were obtained.

The distribution of Q-units obtained by SVTDM was found to reliably describe the compositional dependence of the selected properties of the model borosilicate glass.

Acknowledgments
This work was supported by The Slovak Grant Agency for Science under grant No. VEGA/1/0021/23, 2/0043/25, and by the Research and Development Support Agency APVV-21-0016, APVV-22-0062.

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Thermo-analytical and spectroscopic study of aluminoborosilicate glasses

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Keywords: aluminoborosilicate glass, Raman spectroscopy, glass transition, viscosity multilinear regression

A series of seven aluminoborosilicate glasses was analysed using thermo-analytical and spectroscopic techniques to determine the impact of SiO_2, Al_2O_3, and B_2O_3 on various properties. Multilinear regression analysis was used to quantify the compositional correlation of observed trends. The fundamental physico-chemical properties, including density, refractive index, and molar refractivity, were found to be a linear combination of the contributions from the three network-forming oxides, with additional modifying oxides playing only a secondary role. The amorphous character of the prepared glasses was demonstrated via X-ray diffraction (XRD) analysis, while structural information associated with the bonding arrangements was provided by Raman spectroscopy. The composition of the prepared glasses was determined by X-ray fluorescence spectrometry (XRF). The thermo-mechanical properties, such as glass transition temperature (T_g), were primarily influenced by Al_2O_3 content, with T_g values ranging from 552.3 °C to 580.5 °C (dilatometric) and from 568.3 °C to 601.8 °C (calorimetric) depending on the specific oxide composition. For instance, the base glass had T_g values of 552.3°C (dilatometric) and 577.6 °C (calorimetric), while variations in SiO_2, B_2O_3, and Al_2O_3 content resulted in T_g values such as 580.5°C and 601.8 °C for Si+, and 565.6 °C and 585.6°C for Al+. On the other hand, the properties of viscous flow, including activation energy and kinetic fragility, were predominantly affected by B_2O_3 content.

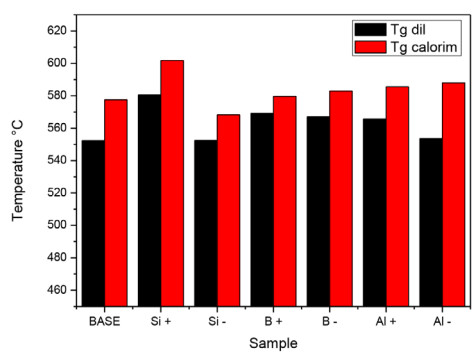

Fig. 1. Comparison of Glass Transition Temperatures (T_g) obtained by Dilatometry and Calorimetry

Acknowledgments
This work was supported by The Slovak Grant Agency for Science under grant No. VEGA/1/0021/23, 2/0043/25, and by the Research and Development Support Agency APVV-21-0016, APVV-22-0062.

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The influence of Li_2O on the structure and thermal properties of Al_2O_3-CaO-K_2O-Na_2O-SiO_2 glass

Aleksandra Nowicka[1], Branislav Hruška[1], Jaroslava Gombarová[1], Hana Kaňková[1], Lenka Buňová[1], Beata Pecušová[1], Anna Prnová[2], Dušan Galusek[1,2], Dagmar Galusková[1]*

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Keywords: glasses, thermal stability, thermal properties, DTA, XRD

This study investigates and compares the structural and thermal properties of glasses in the Al_2O_3-CaO-K_2O-Li_2O-Na_2O-SiO_2 system, varying Li_2O concentrations (0–10 wt.%). The physico-chemical, thermal, and structural properties were analysed. The amorphous character of the prepared glasses was confirmed by X-ray diffraction (XRD) analysis. The differential thermal analysis (DTA) results (Fig.1) show that increasing Li_2O content decreases the glass transition temperature (Tg) from 592°C to 440°C, indicating reduced thermal stability. Moreover, DTA identified dual crystallization exotherms in the range of 584°C to 758°C for samples containing 6 wt.% or more of Li_2O. This phenomenon is associated with the formation of the Li_2SiO_3 phase, as verified by X-ray diffraction (Fig. 2). Fourier Transform Infrared (FT-IR) spectroscopy demonstrated progressive disruption of the Si-O-Si network with increasing Li_2O content. These findings demonstrate Li_2O's dual role as a network modifier and crystallization promoter, critical for tailoring thermal and structural properties in advanced glasses.

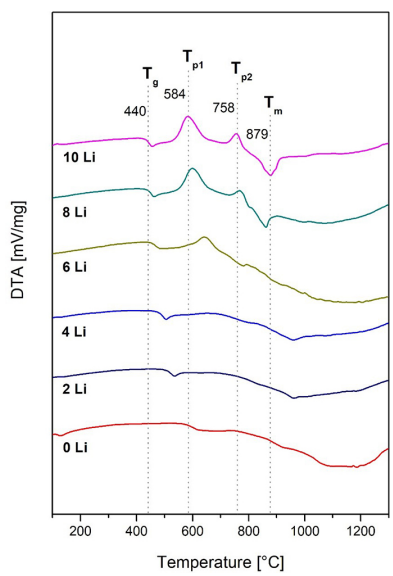

Fig. 1. DTA curve of all samples with marking of thermal characteristics of glasses.

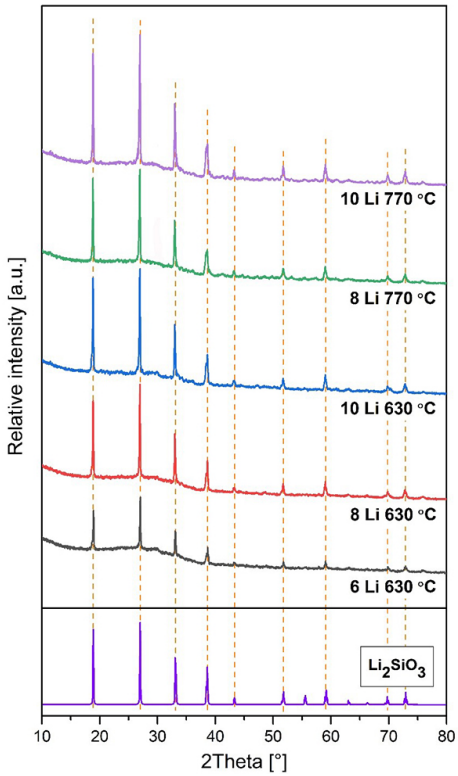

Fig. 2. XRD patterns after heat treatment of selected glass samples.

Acknowledgments

This work was supported by The Slovak Grant Agency for Science under grant No VEGA/1/0021/23 and by the Research and Development Support Agency APVV-22–0062.

Compositional influence on physico-chemical properties of SiO_2-Al_2O_3-B_2O_3 based glassy networks

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Keywords: glasses, thermal properties, alumina-borosilicate glass, glass transition temperature, viscosity

A series of seventeen alumina-borosilicate glasses was studied to identify the influence of the individual oxides. For each network forming oxides, the amount was either increased or decreased by 10 relative mol % from their baseline values (base glass). For the remaining oxides, the content was either increased by 40 relative mol % or reduced to zero. The chemical composition of prepared glasses was analysed by X-ray fluorescence (XRF) analysis. X-ray diffraction (XRD) analysis confirmed the amorphous character of prepared glasses. The structure of prepared glasses was analysed by Raman spectroscopy. The basic physico-chemical properties, such as viscosity, density, glass transition temperature (T_g), coefficient of linear thermal expansion of glass ($10^6\alpha_g$), and coefficient of linear thermal expansion of liquid ($10^6\alpha_l$), were determined. The most significant increase in T_g can be observed in „Si+“ sample. The highest value of the activation energy of the viscous flow (E_η) was observed for „Na +” and the lowest for „Na –“ sample, 557 kJ.mol^{-1} and 419 kJ.mol^{-1}, respectively. Density and molar volume are a linearly additive combination of the roughly equally weighted contributions of the three network-forming oxides. The additional modifying oxides play only a secondary role in influencing these quantities.

Table 1. Thermal properties of studied glasses.

sample	$10^6\alpha_g$	$10^6\alpha_l$	T_g	$E\eta$
	[°C^{-1}]	[°C^{-1}]	[°C]	[kJ.mol^{-1}]
BASE	6.39	40.00	582	538
Si +	3.84	26.39	599	453
Si -	6.85	45.51	569	530
B +	4.83	36.64	585	488
B -	5.38	34.69	579	491
Al +	7.01	31.09	586	487
Al -	5.05	38.41	576	473
Na +	7.43	50.61	576	557
Na -	4.51	24.69	587	419
Ca +	4.81	41.75	578	512
Ca -	4.89	32.57	584	497
K +	3.76	38.15	580	484
K -	5.54	34.73	585	493
Zn +	5.63	32.88	579	491
Zn -	5.54	37.17	583	493
Ba +	6.19	39.95	581	491
Ba -	5.46	33.09	583	478

Acknowledgments

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Correlation between thermal properties and the structure of glass-crystalline ceramic glazes

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Keywords: glass-ceramic glazes, structural properties

The examined glass-crystalline glazes are based on the classic oxide system SiO_2-Al_2O_3-CaO-(Na_2O-K_2O), calcium glazes differing in the type of alkali oxide introduced into the composition, Na_2O or K_2O. The main variable in both groups of the glazes is the ratio of molar ratio of SiO_2/Al_2O_3. On the samples prepared, tests were carried out, including the determination of thermal-technological and structural properties. The most important thermal tests include the determination of characteristic temperatures, thermal expansion coefficients and high-temperature viscosities of glazes. From the structural tests, it is worth mentioning the qualitative and quantitative phase composition XRD supplemented with selected electron microscope images and studies in the mid-infrared range. The results obtained show that, depending on the oxide composition, there are correlations for both types of glazes, CaNa and CaK. However, the influence of the SiO_2/Al_2O_3 molar ratios shows deviations from seemingly logical correlations and is surprising in some cases.

Silicon and carbon multilayer transformation into cubic silicon carbide

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Keywords: phase transformation, silicon carbide, polytype, diffusion, DSC

The integration of high temperature refractory ceramic materials, for example silicon carbide, into silicon semiconductor process technology chains and for other application fields requires low thermal budget processing or alternative routes. Available growth technologies offer temperatures down to 750°C and are based on reactive sputtering, chemical vapor deposition or molecular beam epitaxy. At growth temperature between 700 and 1000°C the growth rates are limited and the growth duration of micrometer thick layers determines the thermal budget. To overcome this issue an alternative method can be applied. It consists in a combination of sputtering a silicon-carbon multilayer stack and subsequent rapid thermal annealing (RTA). Here we investigate the influence of the Si-C bilayer thickness to achieve transformation of the Si-C bilayer stack into SiC.

The Si-C bilayers were deposited using magnetron sputtering of Si and C targets. Alternating layers of Si and C are repeatedly deposited onto a silicon substrate until achieving an overall film thickness of 1 μm. The thickness of the single silicon and carbon layers were 5, 10, 20 and 50 nm resulting in bilayer thicknesses λ of 10, 20, 40 and 100 nm, respectively. The RTA was carried out in a temperature range between 500 and 1100°C in pure argon atmosphere with annealing times ranging from 1 to 5 min. The heating rate was set to 10 K/s. The cooling rate was kept at 4 K/s. The structural investigations were performed by X-ray diffraction (XRD) accompanied by Fourier transform infrared spectroscopy (FTIR) complemented by differential scanning calorimetry. The X-ray diffraction patterns were analysed by Rietveld method to extract the structural properties. Morphological investigations were carried out with scanning electron microscopy (SEM).

During annealing the total layer thickness shrinks. The densification of the layer stack is caused by two factors. Firstly, during ramping the substrate temperature to the final annealing temperature recrystallization of the deposited layer occurs. Secondly, at the interfaces between the silicon and carbon layers SiC was formed by interdiffusion and reaction of silicon with carbon in the interdiffused regions. These processes lead to densification of

the multilayer stack. The shrinkage of the total layer thickness of the multilayer stack was confirmed by FTIR measurements, where a blue shift of the thickness oscillations was observed. Secondly, starting with a bilayer thickness of $\lambda = 40$ nm Si is not fully consumed Si in the Si-C to SiC transformation process. The maximum of the 3C-SiC XRD intensities appears at $\lambda = 20$ nm with no Si peaks indicating on a complete Si-C to SiC transformation. Therefore, it can be concluded that the critical bilayer thickness for a complete transformation is between 20 and 30 nm. The onset of the SiC formation was determined to be around 700°C. For annealing temperatures below 1000°C the SiC was tensile stressed, whereas for higher annealing temperatures compressive stress was obtained. This result was corroborated by FTIR measurements where a change of the 3C-SiC TO vibration frequency from 785 and 800 cm^{-1} was observed if the annealing temperature increases from 800 to 1100°C. The grain size is limited to values smaller than the single layer thickness. A model of the transformation process will be presented.

Fluoroindate glasses: thermal, structural and optical investigations

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Keywords: fluoride glasses, thermal stability, local structure, optical properties

Multicomponent fluoroindate glasses offer some advantages over commercial fluorozirconate glasses (ZBLAN) due to their lower phonon energy, wider infrared transmission window, higher fiber-drawing ability and resistance against devitrification [1,2]. For that reason, fluoroindate glasses are proposed as superior precursor fluoride glass systems for fabrication of next-generation optical fibers and their mid-infrared luminescence applications [3]. Recently, generation of visible light [4] and mid-infrared radiation [5] from fluoroindate glass fibers was successfully obtained. Here, we present thermal, structural and optical properties of multicomponent fluoroindate glasses. In particular, influence of activator (Pr^{3+}, Er^{3+}) concentration and oxide glass-modifier (P_2O_5) content on local structure and thermal stability parameters have been examined using DSC and XRD methods. For low activator concentration, thermal stability parameter defined as difference between glass transition temperature T_g and crystallization onset T_x, is higher than 100°C suggesting the possibility of fiber drawing from precursor fluoroindate glass. With increasing activator concentration stability parameter extremely decreased and several crystalline peaks appeared, what was stated by X-ray diffraction. For low P_2O_5 content, thermally stable and transparent non-crystalline oxyfluoride samples based on InF_3 with relatively high thermal stability parameters were prepared, whereas several diffraction lines due to the InOF polycrystalline phase were identified for higher P_2O_5 content. Optical aspects were also evidenced by luminescence spectroscopy in the visible and near-infrared ranges. Effects of Pr^{3+}/Er^{3+} co-doping on broadband near-infrared luminescence spectra and their long-lived decays observed in fluoroindate glasses have been presented and discussed in details [6].

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Thermal properties of boro-germanate glasses

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Keywords: mixed-network-former glasses, thermal properties, thermal stability, thermal treatment, structure-property relationship

Recently, a large number of the oxide modifiers were tested in order to obtain thermally stable glasses with superior physicochemical properties for numerous multifunctional applications. Previous studies revealed that glass-modifiers give important contribution to the thermal characteristics of inorganic glasses [1]. Further investigations show that thermal and structural changes occurring in glass systems with the presence of various network-former components are also significant. Here, thermal properties of borogermanate glasses belonging to large family of mixed-network-former glass systems have been studied. The mixed network former (MNF) effect is quite well observed in glasses containing more than one network former species [2]. In particular, borogermanate glass with extremely different glass-network-formers B_2O_3 and GeO_2 shows interesting structural properties [3]. The local structure of mixed borogermanate glasses is changed significantly due to compositional changes between two B_2O_3 and GeO_2 network-forming systems. Due to relatively large glass-forming region, structure-property relationship can be determined over a wide B_2O_3:GeO_2 molar ratios. In this work, the results obtained for borogermanate glasses are divided into two parts. The first part presents thermal properties with special regards to glass transition temperatures and thermal stability parameters, which are changed with B_2O_3:GeO_2 molar ratio in chemical composition. The second part contains experimental results for borogermanate glasses after thermal treatment. Preliminary investigations demonstrate that borogermanate glasses are less susceptible to the crystallization during heat treatment process compared to the results obtained previously for germanate glasses modified by TiO_2 [4].

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T05: Cultural heritage

Najran retrofitted earth buildings' insights on sustainability

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Keywords: earth buildings, carbon footprint, Najran.

This research delves into the sustainability and cultural significance of earth buildings in Najran when contrasted with reinforced concrete structures. By delving into document analysis and experimental approaches, the study uncovers a common perception that reinforced concrete homes are often seen as symbols of status, spotlighting the potential for promoting earth buildings as an alternative. This shift in perspective prompts the exploration of innovative strategies for carbon offset projects within the realm of sustainable land use, especially concerning the mitigation of carbon emissions. Recent developmental endeavors within Saudi Arabia, exemplified by projects like the Diriyah Gate Development and the Aseer Region Development, underscore a burgeoning dedication to preserving architectural heritage, highlighting the intrinsic value of earth as a building material. Noteworthy is the significantly reduced embodied carbon footprint associated with earth buildings compared to their reinforced concrete counterparts, positioning them as a sustainable and eco-conscious choice for contemporary construction endeavors. Consequently, the insights gleaned from this study not only fuel a renaissance of earth buildings within the landscape of modern architecture but also contribute tangible solutions to combat climate change and stem the tide of biodiversity loss. Ultimately, these research findings have the potential to serve as a compass for policymakers navigating the intersecting realms of land management and climate change mitigation.

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Physico-chemical techniques and statistical analysis of heritage objects data

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Keywords: neolithic pottery, clay, PCA analysis, thermogravimetry, spectroscopy, LIBS

The study aimed at examining objects of cultural heritage using statistical processing of data acquired through physico-chemical methods. Four late Neolithic pottery sherds from four archaeological sites from Western Romania (Iernut, Soimus, Foeni and Ronat), and clay samples from the same sites [1], were analyzed using (ED)XRF, as well as FTIR, XRD, SEM-EDX and TG techniques. Of all acquired results, the data sets generated by XRF investigation were processed by Principal Component Analysis (PCA) and Hierarchical Cluster Analysis (HCA) to exploit the valuable information contained in the respective samples and uncover potential relationships [2]. The HCA dendograms illustrated the hierarchical relationships between samples of each site, based on the similarity of their chemical composition. The PCA results identified the similarities and differences between clay and sherds samples for each respective site, in terms of oxide composition. A multiple correlation heat map further showed that sites soil could have been used as a source material for manufacturing some types of the studied ceramics. Combined HCA and PCA analysis of XRF spectra proved to be a useful tool to compare the results of the investigated ceramic samples.

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Study of blue pigments used in paintings: insights from thermal and hyphenated analytical techniques

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Keywords: blue pigments, hyphenated techniques, structural analysis, restoration, heritage items

The cultural component has increasingly interacted with sciences such as physics, chemistry, biology and materials science. It is one of the few multidisciplinary fields that bridges the humanities and the exact sciences, offering significant interest due to the broad range of research it encompasses [1].
Pigments are among the most important components found in various archaeological artifacts, works of art, and heritage items. As the methods for obtaining, synthesizing and combining them with different types of binders have advanced, the quantity and the quality of these pigments have increased considerably [1,2].

This paper presents a preliminary study on some of the most important and commonly used types of blue pigments. Ten shades from this category of pigments were selected for structural and thermal characterization. These pigments include both inorganic and organic forms such as: *Ultramarine Ghiaro, Ultramarine Blue Deep, Turquoise dark, Manganese blue, Prussian blue, True blue medium, Sky blue, Real blue, Phthalo blue, Indigo blue*. These pigments will subsequently be mixed with different binders to create viable consolidants used in restoration of different works of art.

Techniques such as thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), Fourier-transform infrared spectroscopy (FT-IR), scanning electron microscopy with energy dispersive X-ray spectroscopy (SEM-EDX) and optical microscopy were employed to characterize the samples. These techniques allow the determination of their thermal behavior at elevated temperatures, their chemical structure, and also, to provide the foundations for the development of an update database for their use in restoration and authentication of various heritage items.

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Characterization of red pigment mixtures with binders used in restorations through hyphenated techniques

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Keywords: conservation, thermal analysis, organic binders, red pigments, structural interactions

In general, research conducted in the field of material cultural heritage implies a strong connection between science and art.

Due of the susceptibility of materials to deterioration, a critical issue for archaeologists and restorers of historically significant artifacts is the identification and understanding of degradation processes affecting these objects [1,2]. Such information is vital for preventing further deterioration and plays a key role in conservation procedures such as cleaning or consolidation [2].

To determine the thermal, structural and morphological characteristics of seven red pigments, the following were analyzed: *Vermilion imitative divolo, Permanent red, Carminrot studienpigment, Burnt Siena, Iron oxide red, Cadmiumrot no.3, Universal red*. Additionally, solutions of various organic binders were prepared, including *rabbit glue, lean egg yolk emulsion, ox gall, boiled linseed oil, oil-in-water emulsion (linseed oil, egg yolk and lavender oil*. Then, the mixtures were applied on glass support.

These scientific investigations are complemented by an examination of the state of preservation of the red pigment belonging to a painting on glass from the 19th century (”The Birth of Jesus Christ”).

The study was conducted using techniques such as TG, FT-IR, digital microscope (VIS) etc., to determine the structure of the pigments, binders and their mixtures, as well as the compatibility and interactions between them, thermal stability and surface morphology in relation to binder interaction.

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Bronze, faiance and unknown: analysis of late bronze age samples from the *Grămurada De La Jupani* site (Susani, Traian Vuia, Timis County, Romania) using thermal, microscopic and spectroscopic techniques

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Keywords: ancient artefacts, TG/DTG/DTA, FT-IR, μRaman, SEM-EDX, XRD

The targeted objects are coming from funerary contexts hosted by a barrow, namely *Grămurada de la Jupani*, situated into western Romania, Susani village, Traian Vuia parish, Timiș county. The excavations here started in 2017 (still ongoing), the tumulus being 4 meters in height and having a diameter of 40 meters.

In 2023 the southern half of the barrow was excavated completely and in the central area a wooden (now mineralized) rectangular structure (Structure no. 1) with its long axis oriented N-S) was researched. This structure/house was practically protected by the mound itself, being the main reason for the tumulus construction. Several compartments/rooms were noticed in this southern sector of the Structure no. 1, hosting five rectangular with rounded corners pits. These pits (C.20, C.31, C.36, C.37 and C.46) were filled, right before the erection of the wooden building, with cremated funerary remains, transforming Structure no. 1 into a real house of the dead. From the absolute chronological perspective, Structure no. 1 can be framed between ca. 1380 – 1280 calBC. The remains deposited in these pits contain ash, charcoal, bone fragments (human and animal) and small jewelry items made, based on a macroscopic analysis, from bone, bronze, faience [1] and gold.

The samples were taken from 11 samples of bronze, faience pieces, along with several objects of unknown make, which were analyzed using SEM-EDX, μRaman, FT-IR, XRD and thermal analysis (TG/DTG/DTA), in order to identify composition and manufacturing technique [2-3].

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T06: Energetic materials

Perovskite-based materials for an application in clou technology

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Keywords: perovskites, CLC, TGA analysis, oxygen carriers

Perovskites represent a fascinating class of materials, characterized by the general formula ABO_3. Due to the ease of synthesis of new materials or modifying the composition of existing ones, it is possible to obtain materials with new properties. Some of the materials with perovskite structure are oxygen deficient, and non-stoichiometric materials, that could be used as oxygen transport membranes or oxygen carriers for the chemical looping combustion (CLC) process. The generation of oxygen vacancies in oxygen-deficient perovskites can be achieved, simply by increasing the temperature or by changing the oxygen partial pressure in the reaction environment. Therefore these materials are promising candidates for a class of CLC process, referred to as Chemical Looping with Oxygen Uncoupling (CLOU). In CLOU process, gaseous oxygen released directly from the oxygen carrier is used for fuel combustion. This approach is particularly beneficial for the combustion of solid fuels, since no direct contact between the oxygen carrier and the fuel particle is necessary. In this research different CLOU strontium perovskite materials were evaluated as oxygen carriers for chemical looping combustion of hard coal by using thermogravimetric analysis. Combustion process was monitored online by using quadrupole mass spectrometer.

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Thermal behavior and compatibility study of dihydroxylammonium 3,4-dinitraminofurazan

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A large number of nitramino-featured energetic salts have been reported and some of them show promising properties. Among them, the dihydroxylammonium 3,4-dinitraminofurazan (HADNAF) is easy to synthesize and shows high calculated detonation performances and acceptable thermal stability. The non-isothermal kinetics parameters of HADNAF including the apparent activation energy (E) and pre-exponential factor (A) of the exothermic decomposition reaction, and activation entropy ($\Delta S^{\neq}$), activation enthalpy ($\Delta H^{\neq}$), activation Gibbs free energy ($\Delta G^{\neq}$) at T_{P0} of the reaction and the critical temperature of thermal explosion (T_b) were obtained by Kissinger's and Ozawa's method, respectively. Additionally, the compatibility of HADNAF with other materials (e.g. TNT, RDX, HMX, B, Mg) was tested by DSC method.

Preparation of high iron containing polyvinylferrocenes burning rate catalyst and their catalytic performance for AP

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Ferrocene derivatives can increase the burning-rate of composite solid propellants when used as burning-rate catalyst. But these small molecular ferrocene catalysts have problems of migration and high mechanical sensitivity. Polyferrocenes were expected to solve these problems. Polyvinylferrocenes with iron contents higher than catocene (GFP) were obtained by the anionic polymerization of vinylferrocene. These polyvinylferrocenes have high iron contents ranging from 24.3% to 26.3%, and decomposition temperatures above 350 °C. No obvious weight loss was observed below 350 °C, which indicated that these polyvinylferrocenes were not easy to volatile before their decomposition. The higher thermal decomposition temperature of mixtures of polyvinylferrocenes and AP decreased from 379.6 °C to 351.7 °C, demonstrating high catalytic decomposition performance. The experimentally obtained values of impact sensitivity test indicated that their sensitivity to impact (10-14%) are much lower than that of GFP/AP system (98%).

Studies on thermal decomposition of fusible insensitive explosive compositions based on 2,4-dinitroanisole and waxes

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Keywords: insensitive explosives, explosive compositions, DSC, thermal decomposition, Friedman method

2,4-Dinitroanisole (DNAN) is a low-melting explosive used in explosive compositions prepared by casting [1-4]. It is obtained in high yield of approximately 90% by methoxylation of 1-chloro-2,4-dinitrobenzene. DNAN has a higher melting point than 2,4,6-trinitrotoluene (TNT), which is more advantageous in the case of explosive compositions stored or used at elevated temperatures. DNAN melts at a temperature below 100 °C, which provides good conditions for the casting of explosive compositions using a melter heated with hot water or steam. 2,4-dinitroanisole is more than twice less sensitive to impact as TNT and has comparable sensitivity to friction. Unfortunately, despite better insensitivity to external stimuli, 2,4-dinitroanisole has weaker detonation parameters than TNT [5-6]. One of the most promising high-performance secondary explosive is 4,10-dinitro-2,6,8,12-tetraoxa-4,10-diazatetracyclo-[5.5.0.$0^{5,9}0^{3,11}$]dodecane (TEX), high density secondary explosive, suitable for inclusion in insensitive explosive preparations [7-8]. Thermal decomposition characteristics and thermal sensitivity of explosives reflect the safety of their production, storage, transport and use. Four explosive compositions based on DNAN/TEX/wax were made. The reference material was the DNAN/TEX 35/65 mixture. Samples containing three types of waxes were tested: rice, carnauba and ozokerite. Research was carried out using differential scanning calorimetry (DSC) with 5 different heating rates β = 1, 2, 4, 8 and 16 °C/min. Kinetic calculations were performed using the Friedman method using the NeoKinetic software from Netzsch. The activation energy and pre-exponential factor for the initial conversion degree (α = 0.05) of the wax-free sample were E_a = 200 kJ/mol and $LogA$ = 16.8, respectively. The influence of the addition of 7% wax on the decomposition kinetics parameters was examined.

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Driving towards a greener future: the environmental impact of connected vehicle technologies

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Keywords: V2X communication, connected vehicle, sustainability

This paper analyses the environmental effects of Connected Vehicle (CV) technologies, specifically focusing on Vehicle-to-Everything (V2X) communication. The main advantages of V2X communication include improved safety, better transportation system management, increased mobility, higher efficiency, and reduced emissions. By sharing data, CVs can improve vehicle safety, lower energy use, and decrease emissions. V2X communication can help reduce traffic congestion and improve traffic flow, leading to more efficient road use, lower fuel consumption, and fewer emissions. Traffic flow management techniques, like communicating with traffic signals, can reduce idling and other sources of vehicle-related emissions. Vehicle-to-Vehicle (V2V) communication supports smoother driving patterns, such as cooperative adaptive cruise control, which helps reduce fuel use and emissions.

Sustainable transportation is key to leaving a healthy planet for future generations. V2X can play an important role in this by making roads safer and less congested, which reduces CO2 emissions. Cooperative driving can shorten travel times and reduce sudden accelerations. V2X can also help protect cyclists, encouraging more people to cycle. Additionally, giving priority to public transportation through V2X can increase its use and lower its emissions.

T07: Energy conversion and storage

Thermocline energy storage for enhancing the thermal performance of a hybrid compression-absorption cooling machine powered by a Linear Fresnel CSP system

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Keywords: thermocilne heat storage, Absorption Refrigeration System (ARS), hybrid cycle, solar COP, Linear Fresnel concentrator

Hybrid absorption cooling systems [1] present an attractive solution for valorizing industrial thermal waste, harnessing renewable energy sources, and reducing greenhouse gas emissions. However, their industrial deployment remains limited due to several technical challenges, notably the intermittency of thermal resources and the inadequacy of suitable heat source temperatures. Consequently, ensuring continuous operation and economic profitability remains a challenge.

To address these technical barriers, we propose in this work the integration of a sensible heat storage tank based on the thermocline concept and filled with natural quartzite rocks [2]. Our study focuses mainly on the coupling modalities between the storage tank and a double-effect hybrid compression-absorption refrigeration system using LiBr/H2O pair and powered by a Fresnel-type solar concentrator [3]. In first, we develop a comprehensive dynamic simulation code that accounts for multiple physical and heat-mass transfer phenomena occurring within the system while addressing the challenge of solar energy intermittency. Using real solar and climatic data, this global model provides accurate predictions of the system's response on daily, monthly, and annual scales under realistic dynamic conditions.

For the single-day operation simulation, results show that despite daily variations in incident solar radiation, the integration of the storage tank ensures stable and continuous cold production. The cooling capacity remains constant throughout the day. Depending on the storage volume, it can partially cover night-time demand. The solar COP [6] (ratio between cold production and total incident solar energy) varies between 0.7 and 0.9, while the discharge efficiency ranges from 60% to 70%. However, for the day-to-day operation scenario, simulations reveal that the system's overall performance declines over successive cycles before stabilizing after eight operating cycles (eight days). Analysis of the storage tank behaviour shows that thermal cycling significantly increases the thermocline height, thereby degrading

storage performance. This degradation results in a 20% reduction in discharge efficiency and a 10% decrease in storage tank autonomy, leading to a substantial performance gap between the single-day operation scenario and the day-to-day operation scenario.

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Steam turbine condenser cooling tubes analysis after hp&ip steam bypass modification

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Keywords: bypass modification, condenser, cooling tubes, reconstruction, steam flow, vibration

During reconstruction of the turbine condenser was carried out, incorporating bypass pipelines that direct steam from the boiler directly into the turbine condenser. These steam bypass pipelines are primarily used during boiler start-ups and turbine trips and are equipped with steam dump devices to reduce steam pressure and temperature before entering the condenser. The efficiency and reliability of a steam turbine condenser depend significantly on the performance of its cooling tubes. The condensation system converts the steam from the final turbine stage into condensate, which is then returned to the boiler supply system. The steam undergoes condensation in the condenser. The condensate is pumped through the ejector cooler by one of two condensate pumps, with the other as a backup.

The reconstruction of the turbine condenser with the steam bypass system has introduced new thermal and mechanical stresses on the turbine condenser cooling tubes. Without proper mitigation, these stresses could lead to further failures and reduced condenser efficiency. Implementing optimized spray water control, material enhancements, and continuous monitoring will help improve system reliability and prevent damage. Following the reconstruction of the turbine condenser with steam bypass system, an analysis was conducted to evaluate the condition of the condenser cooling tubes and identify potential issues arising from the operational changes. The analysis of the turbine condenser cooling tubes was conducted based on visual inspection of cooling tubes, assessment of tube material degradation due to thermal and mechanical stresses, operational data review, spray water effectiveness, etc.

To ensure the normal future operation of the turbine condenser, a simulation model of the turbine condenser with the newly installed steam bypass system was developed using computational fluid dynamics techniques. A 3-D model was developed to assess steam flows and velocities in the condenser region to look at impact on cooling tubes.

The analysis results showed that steam velocity in certain areas of the turbine condenser exceeded the critical threshold for vibration, indicating a high risk of vibration-induced damage to the cooling tubes.

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Thermal management optimisation in ab_2 metal hydride storage: dynamic analysis of hydrogen absorption and desorption

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Keywords: hydrogen storage, metal hydrides, dynamic characterisation, thermal management, hydrogen absorption and desorption

Hydrogen is considered a promising fuel for the future due to its high energy density and zero emissions when used in fuel cells, combustion engines, and industrial processes [1]. However, its efficient storage remains one of the main technological challenges [2]. Metal hydrides offer an attractive alternative to high-pressure and cryogenic hydrogen storage methods, as they enable safe and compact storage at moderate pressures and temperatures. The absorption of hydrogen into metal hydrides is an exothermic reaction, whereas desorption requires heat input [3]. Effective thermal management is therefore essential to ensure rapid absorption and desorption kinetics, stable performance, and prolonged lifespan of metal hydride storage systems [4].

As part of the research, dynamic characterisation of hydrogen absorption and desorption was conducted in commercially available AB_2-type metal hydride storage systems within a temperature range of 11 – 55 °C. An effective thermal management solution was designed and experimentally validated, ensuring efficient cooling during absorption and heating during desorption. Additionally, a cooling system was developed and implemented, with its efficiency verified through measurement.

During the experiments, key parameters were recorded, including pressure (0 – 35 bar), metal hydride temperature (11 – 50 °C), gas flow rate, temperatures on the pressure vessel measured using thermocouples, and cooling water temperature. Based on these data, PCT diagrams, time dependencies of gas flow and pressure, filling and emptying times of the storage system, as well as the thermal energy released or consumed during individual processes, were evaluated.

Dynamic characterisation was carried out at a constant cooling water temperature, while the metal hydride temperature varied naturally depending on absorption and desorption. Heat generated during absorption and consumed during desorption caused temperature fluctuations in the pressure vessel, enabling the identification of critical points for optimising thermal management. The analysis determined several parameters, including the maximum reversible hydrogen storage capacity (180 g per storage unit) with a relative capacity of 1.73 wt%, as well as equilibrium pressures ranging from 0 – 30 bar for absorption and 0 – 35 bar for desorption.

The proposed solution was compared with available literature and analysed in terms of potential innovations and improvements. Alternative methods of cooling and heating metal hydride storage systems were also discussed, along with their suitability for various applications in the hydrogen economy. The results obtained can be used for further optimisation of hydrogen storage in metal hydride systems.

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Autonomous desalination unit using solar photovoltaic energy: a sustainable approach for water purification

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Water scarcity is one of the most pressing global challenges, especially in remote desert villages and mountainous communities, where access to clean drinking water is limited. Traditional desalination methods rely on fossil fuels, making them costly, energy-intensive, and environmentally unsustainable. To address this issue, we developed an Autonomous Desalination Unit Powered by Solar Photovoltaic (PV) Energy, designed to provide a portable, off-grid, and eco-friendly solution for water purification.

The unit integrates solar PV panels, natural filtration, reverse osmosis (RO), and UV sterilization, ensuring an efficient, self-sustaining water purification process. The system was designed and validated through CAD modeling, theoretical calculations, and simulations, optimizing energy use while maintaining water quality standards. The autonomous nature of the unit allows it to function with minimal human intervention, making it particularly suitable for isolated communities and disaster-stricken areas.

Findings from our design and simulations demonstrate the feasibility of a sustainable, scalable desalination system that operates independently of conventional power sources. The portability of the unit makes it adaptable to various terrains, ensuring that clean water can be delivered to people in long-distance remote areas. Our work is motivated by the United Nations Sustainable Development Goals (SDGs), particularly SDG 6 (Clean Water and Sanitation) and SDG 7 (Affordable and Clean Energy), aiming to promote sustainable water access while reducing dependence on nonrenewable energy sources.

Future improvements focus on enhancing brine waste management, increasing scalability for larger applications, and integrating IoT-based remote monitoring for better operational efficiency. Accordingly, the present research represents a step toward sustainable, decentralized water solutions, contributing to a cleaner and more equitable future. It is envisioned that this method is a sustainable approach for water purification.

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Sustainable thermal management via transportable heat storage units

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Keywords: waste heat recovery, mobile heat storage

Environmental protection has become an essential and unavoidable topic in recent years, particularly in the industrial and energy sectors. Increasing energy efficiency and reducing harmful emissions are among the most effective tools to achieve sustainability goals. One practical approach is the utilization of waste heat generated during manufacturing and energy production. However, a major challenge lies in the temporal and spatial mismatch between heat availability and demand, making immediate utilization unfeasible. This research investigates a mobile heat storage unit capable of temporarily storing waste heat and later transporting it for reuse—such as integrating it into a building's heating system. While similar international attempts have often failed due to high transportation costs and environmental impact, the proposed concept addresses these issues by focusing on precise demand assessment, short transport distances, and low-emission transportation methods. The study includes the analysis of a specific waste heat source and a corresponding consumer, with the goal of sizing the storage unit and selecting appropriate transport equipment based on technical, environmental, and economic criteria. Special emphasis is placed on quantifying potential energy savings, emission reductions, and cost-efficiency, as well as calculating the investment’s return.

Thermal energy storage systems: particle swarm optimization-driven approach for improved performances and operational reliability

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Keywords: thermal energy storage systems, Particle Swarm Optimization, design parameters, performances

The development of efficient thermal energy storage (TES) systems is crucial for enhancing the performance of renewable energy applications, particularly in concentrating solar power (CSP) plants. Thermocline storage, characterized by a packed bed of solid particles and heat transfer fluids (HTFs), offers a cost-effective solution. However, the performance of these systems is highly dependent on design parameters such as storage tank geometry, HTF mass rate, and thermal stratification stability. In this context, Particle Swarm Optimization (PSO) emerges as a relevant method for optimizing thermocline storage system performance by simultaneously considering multiple design and operational parameters [1, 2]. The present study aims to deploy the PSO algorithm to optimize thermocline thermal storage systems by identifying the best configuration for maximizing energy efficiency, minimizing pumping energy, and enhancing system autonomy. Key performance indicators include geometric characteristics of the storage tank, the packed bed porosity, the pumping energy requirements and the charge/discharge associated efficiencies and performances. A thermocline storage model was developed based on transient heat transfer equations under non-local thermal equilibrium conditions [3]. The PSO algorithm was applied to optimize critical parameters such as porosity (0.05–0.6), particle size (0.005–0.02 m), tank height (2–7 m), total volume (10–30 m³), and mass flow rate (0.5–5 kg/s). The objective functions targeted overall system efficiency by balancing charge and discharge performance while minimizing energy losses. Different HTFs (Hitec XL, Syltherm, Colza Oil, etc.) were considered to evaluate their impact on thermal performance. As a result, the optimized thermocline storage system achieved a maximum overall efficiency of 63.1% when prioritizing discharge, demonstrating significant improvements in energy utilization. The optimization process led to a considerable reduction in charging and discharging times, reaching 2.78 hours and 2.55 hours, respectively, in the most efficient configurations. Additionally, the highest energy absorbed by the heat transfer fluid (HTF) during discharge was recorded at 7122 MJ, highlighting the system's capability for efficient thermal energy recovery. Pumping energy requirements were also minimized, with reductions of up to 80% in specific configurations, leading to lower operational costs and enhanced system sustainability. Furthermore, the study identified the optimal tank geometry, including particle size and porosity, to maximize thermal stratification while maintaining stable fluid flow dynamics. This optimization contributed to an improved system

autonomy by effectively balancing charging and discharging efficiencies, ensuring reliable energy availability over extended operational cycles. Overall, by leveraging PSO, this study provides an advanced methodological approach for designing high-performance thermocline storage systems, ensuring both operational reliability and enhanced energy efficiency. The findings contribute to the ongoing development of optimized thermal storage technologies for large-scale energy applications, supporting the integration of renewable energy sources with improved storage solutions.

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Optimizing cogeneration plant performance for sustainable energy in multi-energy demand industries

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Keywords: marine engine, bulk carrier, entropy, irreversibility, sustainability

Optimizing cogeneration plant performance for sustainable energy, particularly in the context of decarbonization, necessitates a multifaceted approach that balances efficiency gains with reduced reliance on fossil fuels. This involves not only improving the thermodynamic efficiency of the plant itself but also evaluating and potentially modifying the energy-intensive industrial processes it serves, encouraging the use of renewable energy sources, and implementing strategies for capturing and utilizing waste heat more effectively. This study investigates the environmental impact of industrial cogeneration plants, a supported solution for sustainable energy in multi-energy demanding facilities. Despite their efficiency, fossil fuel consumption in these plants often leads to significant environmental pollution. In the study, the real operational data from an industrial cogeneration plant was utilized, and employed an entropy-based irreversibility analysis to assess environmental impacts, focusing on two key indicators of pollution potential. Results indicate an average overall efficiency of 62.01% for the plant's processes but highlight a substantial thermal irreversibility effect. The analysis concludes with recommendations for optimizing the operational performance of cogeneration processes to enhance their environmental sustainability.

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Evaluations of plant-based dielectric fluids for transformers: performance, stability, and sustainability

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Keywords: plant-based dielectric fluid, esterification, voltage tolerance, heat of combustion, kinematic viscosity, thermal stability

This study evaluates the feasibility of using plant-based dielectric fluids for transformer applications, focusing on their environmental performance and thermal stability. As efforts to reduce greenhouse gas emissions increase, plant-based fluids emerge as eco-friendly, biodegradable alternatives to traditional mineral oils [1]. In the research, soybean and canola oils were esterified with methanol, ethanol, propanol, and butanol. Among the samples tested, soybean oil methyl ester exhibited the highest voltage resistance [2], measuring 64.90 ± 9.74 kV, highlighting its potential for electrical applications [2]. Its acid value was 0.0228 ± 0.0006 mg KOH g^{-1}, meeting the dielectric fluid standard of less than 0.03 mg KOH g^{-1}, ensuring long-term stability. Regarding heat of combustion, soybean oil fatty acid methyl ester demonstrated approximately 20% of the energy density of mineral oil. While this value is lower, its environmental and biodegradability advantages are significant. Kinematic viscosity testing at 40°C showed that soybean oil methyl ester has superior flowability at 4.4186 ± 0.0235 $mm^2\ s^{-1}$ compared to commercial dielectric fluids, which measured 8.7342 ± 0.0447 $mm^2\ s^{-1}$ [2]. This makes soybean oil ideal for high-efficiency heat transfer applications. Nanoparticles were incorporated into soybean oil methyl ester to enhance its dielectric properties [3]. Tests on breakdown voltage, thermal stability, and high-temperature performance utilized advanced instruments, including a dielectric breakdown voltage tester, oxygen bomb calorimeter, differential scanning calorimetry (DSC), and isothermal calorimeter (TAM Air). The results demonstrated that adding nanofluids improved thermal conductivity while maintaining desirable dielectric properties [1–6]. Overall, soybean oil methyl ester meets key standards for dielectric fluids and offers excellent fluidity, making it suitable for insulating power equipment. This study is a valuable reference for developing sustainable plant-based dielectric fluids, which show significant potential for future power systems.

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Investigating CO_2 capture and sequestration *via* volumetry, thermal analysis, and calorimetry

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Keywords: CO_2 capture, CO_2 adsorption, volumetry, thermogravimetric analysis, differential scanning calorimetry, calorimetry

The growing concentration of anthropogenic CO_2, primarily from fossil fuel combustion and industrial processes, has led to intensified research in carbon capture, utilization, and storage. This study investigates CO_2 capture using a combination of volumetry, thermal analysis (TGA/DSC), and calorimetry to understand the sorption properties and energetics of various materials.

Volumetric experiments were conducted to quantify CO_2 uptake under controlled temperature and pressure. Notably, periodic mesoporous organosilica with ethylene bridges (PMO-Ethane) demonstrated a high reversible adsorption capacity of 827.8 $mg \cdot g^{-1}$ at 0 °C and 34 bar, maintaining stability over 10 cycles [1]. Additional volumetric tests on coal-based sorbents revealed significant capacity enhancement through surface modification: methyl orange–primed sub-bituminous coal reached 18.7 $mol \cdot kg^{-1}$ CO_2 at 50 °C and 37 bar, a drastic improvement over unmodified coal (1.95 $mol \cdot kg^{-1}$) [2]. These results emphasize the importance of material surface chemistry and pore structure.

Thermal analysis using thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) was carried out to investigate the CO_2 and H_2O adsorption behavior of three honeycomb carbon monoliths (793, 932, and AM03) under conditions simulating cement flue gas. At 50 °C, CO_2 showed rapid adsorption kinetics, reaching equilibrium within 2 minutes, while H_2O adsorption was slower, taking up to 25 minutes to stabilize. Among the tested samples, monolith 793 achieved the highest CO_2 selectivity, demonstrating □1 $mmol \cdot g^{-1}$ adsorption capacity with favorable kinetics at 50 °C in a gas stream containing 32 vol % CO_2 and 4 vol % $H_2O_{(v)}$ at 101.3 kPa, confirming its strong potential performance in humid industrial environments [3].

Calorimetric analysis, performed with a Setaram C-80 calorimeter, was used to determine the heat of CO_2 absorption in amine-based solvent systems. Aqueous 30 wt% monoethanolamine solutions modified with monoethylene glycol (MEG) showed variable absorption thermodynamics. At 40 °C, the addition of MEG increased the heat of absorption and CO_2 solubility, while at 120 °C, the reduced heat favored easier desorption, contributing to energy savings in solvent regeneration cycles [4]. In the solid phase, mesocellular silica foams (MSU-F) impregnated with tetraethylenepentamine (TEPA) and diethanolamine (DEA) showed high CO_2 uptake: up to 5.91 $mmol \cdot g^{-1}$ at 50 °C and 100 kPa, and tunable heats of adsorption ranging from 68 $kJ \cdot mol^{-1}$, to 104 $kJ \cdot mol^{-1}$, depending on the DEA/TEPA ratio [5].

This comprehensive study demonstrates how integrating volumetry, thermal analysis, and calorimetry enables robust characterization of CO_2 sorption behavior. These methodologies are essential for selecting and optimizing materials for efficient, reversible, and low-energy CO_2 capture in real-world applications.

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Properties of porous materials from carbonised biomass infiltrated with PE G6000 modified with graphene

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Keywords: phase change materials, thermal analysis, DSC, shape stabilization, PEG 6000

Organic phase change materials (PCMs) have attracted significant attention from researchers for many years, particularly due to their high energy storage capacity [1,2]. However, a key limitation of PCMs is their solid-liquid phase transition, which causes a volume change and poses a risk of leakage. Additionally, the inclusion of nanoparticles can lead to sedimentation, disrupting uniformity during the initial heating cycle [3].

PEG 6000 has been selected because it interesting properties as a PCM [4] and, according to our previous research, it showed minimal leakage during testing.

Various methods for stabilizing PCMs are described in the literature, including the use of polysaccharides [5] or porous carbon materials derived from the carbonization of specific fruit peels, such as watermelon or orange peels [6,7].

The primary objective of our research was to develop a shape-stabilized PCM. To achieve this, we prepared PEG 6000 as PCM enhanced with graphene and incorporated it into carbonized fruit peel that had been modified with graphene. The properties of the resulting PCM composites were analyzed using differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), and scanning electron microscopy (SEM). Additionally, we calculated the percentage of PCM within the carbonized fruit biomass.

Acknowledgments
This work was supported from the subsidy of the Ministry of Education and Science for the AGH University of Science and Technology in Kraków (Project No 16.16.160.557). Research project partly supported by program „Excellence initiative – research university" for the AGH University of Krakow.

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The impact of inner tube shape on the performance of a hexagonal porous thermal energy storage unit loaded with nepcm

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Keywords: Latent Heat Storage (LHS), double-diffusive, nano-encapsulated phase change material, porous media

The recovery of lost heat and the optimization of heat transfer rates are of significant interest to engineers and scientists because of their direct influence on global warming. This article presents a numerical endeavour to enhance the thermal efficiency of a Latent Heat Storage (LHS) system. The double-diffusive convection of Nano-encapsulated phase change material (NEPCM), situated in an annulus between an inner Koch snowflake cylinder and an outside hexagon, is analyzed using the Galerkin Finite Element Method (GFEM). The research encompasses a wide array of parameters, including Rayleigh numbers ($Ra = 10^3$ to 10^6), Darcy numbers ($Da = 10^{-2}$ to 10^{-5}), Lewis numbers (Le = 0.1 to 5), and the geometry of the inner cylinder (triangular, Koch snowflake). The results indicated that elevating Ra and Da substantially enhanced the heat transfer rates, but the effect of Le was rather little. At the maximum examined Ra, elevating Da to 10^{-5} enhanced the heat transfer rate by 160%, whereas an increase in Le to 5 resulted in a 22% reduction. Furthermore, it was observed that the triangular body has a superior heat transfer rate relative to the other two forms. The triangular configuration yielded a 116% increase in the heat transfer rate relative to the snowflake configuration.

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T08: Exergy, experimental thermodynamics

Solubility and thermodynamic function of carbamazepine-saccharin co-crystal in ethanolic solution

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Keywords: solubility, co-crystal, carbamazepine, saccharin

The article is assessing the solubility and thermodynamic function of carbamazepine-saccharin co-crystal in varying saccharin concentrations in ethanolic solution and temperatures. Solubility of carbamazepine-saccharin co-crystal were determined by synthetic and high-performance liquid chromatography methods. The solubility obtained was correlated well with van't Hoff model and was found to increases as temperature rises for all conditions studied. The solubility values of the co-crystal were higher than the carbamazepine solubility, thus indicate the solubility has improved with the formation of co-crystal at the studied temperatures. Based on the apparent thermodynamic analysis parameter, it was indicated an endothermic and entropy-driven dissolution of CBZ-SAC co-crystal. From the results, carbamazepine-saccharin co-crystal has been considered freely soluble in ethanol solution with non-SAC excess.

Acknowledgments
The research was funded by the Ministry of Higher Education under Fundamental Research Grant Scheme No. FRGS/1/2018/TK05/UMP/02/7 (RDU190182). The authors would like to acknowledge Universiti Malaysia Pahang Al-Sultan Abdullah for the laboratory equipment and facilities.

Cfd simulation for co-gasification of coal blended with biomass in an one-stage oxygen-blown entrained bed co-gasifier

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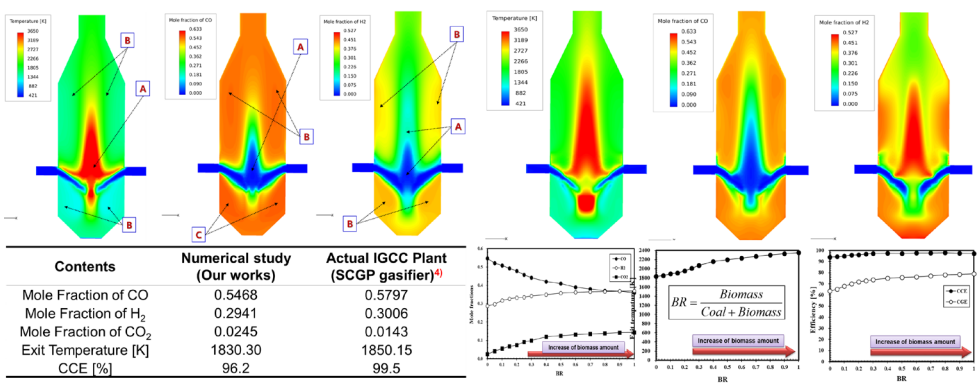
Keywords: type your, keywords here, separated, with commas

Since detailed empirical characterization of any gasification process is difficult due to high heating rate and short residence time, numerical simulation has been recognized as one of the most important requirements for advancement of gasification technology. Computational fluid dynamics (CFD) analysis provides results for the prediction of fluid flow and species concentrations in the gasifier with considerations of reactor geometry and operating conditions [1]. In this study, CFD modeling on co-gasification of coal blended with biomass in an one-stage entrained bed gasifier (Shell Coal Gasification Process gasifier) was performed. Parametric studies with biomass-to-coal blending ratios (BR: 0~0.2), steam/fuel ratios (0.008~0.075), and O2/fuel ratio (0.75) were carried out using a commercial code, ANSYS FLUENT. CFD modeling of gas-phase was conducted by solving the steady-state Navier–Stokes, energy, and species transport equations. Gas-phase chemical reactions were solved via the Finite-Rate/Eddy-Dissipation Model. All coal-biomass particles were treated as discrete, secondary phase dispersed in the continuous phase via the Discrete Phase Model with the stochastic tracking to consider the turbulent dispersion effect.



Contents	Numerical study (Our works)	Actual IGCC Plant (SCGP gasifier)[4]
Mole Fraction of CO	0.5468	0.5797
Mole Fraction of H_2	0.2941	0.3006
Mole Fraction of CO_2	0.0245	0.0143
Exit Temperature [K]	1830.30	1850.15
CCE [%]	96.2	99.5

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Assessment of engine thermal efficiency in relation to angle of attack: a digital twin-based approach

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Keywords: digital twin, engine performance, simulation

One of the most important parameters for evaluating engine performance in the aviation industry is thermal efficiency, which has a direct impact on fuel consumption and operational cost. Optimizing thermal efficiency helps to reduce the amount of fuel required for flight ranges and reduce emissions. It is therefore of critical importance due to its impact on the targeted parameters of sustainability, low cost and high performance in aviation.

In this paper, the effect of angle of attack variation on thermal efficiency in a regional cargo aircraft with turboprop engine is investigated. In order to evaluate the system as a whole and examine the performance values in detail, a digital twin of the aircraft is modelled. On this twin, the engine performance is simulated at different angles of attack and the effect on the thermal efficiency of the engine is explained graphically. The aim of this study is to provide a basis for understanding the effect of angle of attack on thermal efficiency and optimizing it with real-time data.

T09: Fuels, biofuels

Solar driven pyrolysis for the production of biofuels: an experimental study

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Keywords: pyrolysis, solar energy, biomass, syngas, biofuel, GHG, bio-oil

The pyrolysis of biomass employing solar energy for the production of biofuels is covered in detail in this study. Bioenergy has emerged as major short- and medium-term alternative to fossil fuels, presenting a substantial promise for decreasing greenhouse gas (GHG) emissions as the world's energy demand continues to rise fast and fossil fuel stocks continue to deplete. The most practical technique for converting biomass into biofuels is believed to be thermo-chemical conversion. Combustion, torrefaction, pyrolysis, hydrothermal liquefaction, and gasification are applicable methods used in this process. Three main products are typically produced by the pyrolysis in particular: bio-oil, biochar, and syngas. Under this investigation, solar cells were used to power the pyrolysis reactor, which pyrolysed biomass. Temperatures between 350 and 550 °C were used for the pyrolysis process, which was carried out under various operating conditions. Using the slow pyrolysis process, about 27% bio-oil and 43% biochar were produced in the products. Furthermore, the impact of several catalysts on the pyrolysis process was examined. Results revealed that the use of a catalyst improved the yield and quality of the bio-oil. A temperature of 550 °C was found to be the optimum operating condition, yielding the largest amount of bio-oil.

Acknowledgments
The researchers would like to acknowledge the assistance provided by the South African National Energy Development Institute (sanedi) for funding the project. This project has received funding from the European Union's Horizon 2020 Research and Innovation Programme under Grant Agreement 963530.

Application of digital twin technology for the analysis of combustion emission of fuel blends

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Keywords: fuel blends, digital twin method, emissions

In recent years, developments in digital twin technology have significantly contributed to environmental sustainability and energy efficiency research through its simulation and real-time monitoring capabilities. The evaluation of emission performance from alternative fuel blends is particularly crucial for energy management and climate change mitigation in the aviation sector. In this context, digital twin technology provides an innovative framework for modelling complex combustion dynamics and developing emission reduction strategies. This study developed a virtual engine model of a gas turbine aircraft engine using the digital twin approach, systematically investigating the emission characteristics of different fuel blends. The performance parameters of the compressor and turbine components were modelled based on component data and the accuracy of the digital twin model was confirmed using real-time sensor data. Under optimal flight conditions, combustion processes of fuel blends with varying mixture ratios were simulated. Comprehensive parametric analyses were systematically performed to quantify the influence of critical operational parameters—including fuel composition, combustion temperature, and air-fuel ratio—on emission characteristics. A detailed comparative assessment of emission profiles was conducted across varying fuel blend ratios. The experimental results demonstrate that digital twin technology serves as a reliable method for characterizing emissions in fuel blend combustion research. This innovative methodology facilitates accelerated virtual scenario testing while demonstrating considerable potential as a predictive decision-support platform for clean energy transition strategies. The ability of this technology to analyse and optimise the emission characteristics of sustainable aviation is particularly noteworthy, as it will generate the necessary data for the development of environmentally responsible fuels.

The effect of hydrothermal processing temperature on the characteristic of hydrochars obtained from apple pomace

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Keywords: apple pomace, hydrochar, hydrothermal carbonization

Poland is one of the leading apple producers in Europe, which substantial part is further processed into food products such as juices and nectars. The food processing industry generates considerable amounts of waste characterized by high moisture content (such as pomace, lees, and sediments). It is estimated that globally, apple processing results in the production of 3 to 4.2 million tons of pomace annually [1]. Currently, only a limited part of this waste finds sustainable applications, such as a raw material for biogas production, while the majority is composted, incinerated, or landfilled. These methods are not optimal in terms of a circular economy and contribute to increased greenhouse gas emissions. The high water content in waste generated by the food processing industry promotes the growth of microorganisms that are hazardous to humans and animals. When such waste is stored in landfills, uncontrolled anaerobic decomposition may occur, leading to the release of methane into the environment. An alternative thermochemical processing method for wet waste is hydrothermal carbonization (HTC), in which water serves as the reaction medium. The process is aimed at the formation of hydrochars, which are carbon-based materials exhibiting a wide range of applications. They can be used, among others, as solid biofuels, catalyst supports, electroactive components in electrochemical devices, or as an alternative to activated carbon in sorption processes and water purification [2].

In this study, the effect of HTC temperature on the properties of the obtained hydrochars was analyzed. Apple pomace was subjected to carbonization at temperatures ranging from 150 °C to 300 °C for 4 hours, with a mass ratio of the pomace to water of 1:4. The hydrochar yield varied between 51.6 wt.% and 33.7 wt.% at 150 °C and 250 °C, respectively. At 300 °C, an increase in hydrochar yield was observed, reaching 36.1 wt.%. This is likely caused by the formation of solid products from secondary reactions occurring in the aqueous phase. The comparative characterization of hydrochars was conducted by means of Fourier-transform infrared spectroscopy (FT-IR), surface area and pore volume determination based on the Brunauer–Emmett–Teller (BET) method, elemental and proximate analysis of the resulting hydrochars. In order to assess the distribution of carbon between the process water and the hydrochars, total organic carbon (TOC) analysis of the aqueous phase (process water) was also conducted. The HTC process temperature notably influences the surface properties of hydrochars. The specific surface area was observed to vary with carbonization temperature, ranging from 7 m^2/g to 33 m^2/g. It was found that increasing the temperature leads to a reduction in organic carbon content in the process water, which may indicate the repolymerization of furan compounds (such as 5-hydroxymethylfurfural) at higher temperatures and their subsequent incorporation into the hydrochar structure. This observation is further supported

by the secondary increase in hydrochar yield observed at 300°C. This process can influence the properties of the obtained hydrochars, including porosity, the nature of surface functional groups, and total carbon content. The conducted research demonstrated that temperature is a key parameter in the HTC process, determining the properties of the derived hydrochars. Proper temperature selection allows for precise control over the final product characteristics, enabling its application in a wide range of fields, i.e. from solid biofuels to carbon materials serving as precursors for adsorbents or catalyst supports.

Acknowledgments
Research supported by program ‘Excellence initiative – research university” for the AGH University of Krakow (IDUB-4/6261).

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Activity of amorphous NiB/SiO_2 in hydrotreating model reaction: hydrodenitrogenation of carbazole

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Keywords: NiB/SiO_2, Ni_3S_2, hydrodesulfurization (HDS), hydrodenitrogenation (HDN) reaction, carbazole, hydrogenation, metallic Ni^0

The emission of SO_2 and NO_x related to the combustion of transport fuels is still an important aspect from the point of view of the purity of fuels such as gasoline and diesel oil. The current restrictions related to environmental protection force a significant reduction of sulfur and nitrogen content in transport fuels to the lowest possible level [1-3] and even to the level of <1ppm in the case of sulfur [4,5]. Thus, the hydrodesulfurization and hydrodenitrogenation processes are important processes in a modern refinery. It is well known that nitrogen compounds inhibit the HDS reaction and thus make it difficult to desulphurize the raw material to the sulfur content required by the restrictions [6]. Thus, the rapid removal of nitrogen compounds (HDN) at the same time facilitates the removal of sulfur from the feed. Various nitrogen compounds occur in non-hydrotreated diesel fuel, among them quinoline and carbazole derivatives are the least reactive [7]. The hydrodenitrogenation reaction requires hydrogenation of both the ring containing the nitrogen heteroatom and the adjacent aromatic ring before removing nitrogen as NH_3 [7,8]. Therefore, from the HDN point of view, the catalysts should have better hydrogenation properties and, at the same time, be thioresistance to the presence of sulfur in the raw material. Transition metal borides, both bulk and supported on various supports, have very attractive catalytic properties, especially of many hydrogenation reactions [9]. They show higher activity than Raney nickel **[10].** Basically, they are obtained by using a transition metal salt reduction method mainly of nickel and cobalt with $NaBH_4$ or KBH_4 solution [10,11]. The interest in amorphous NiB bulk or supported stems not only from their high catalytic activity and selectivity in hydrogenation reactions but also from their high resistance to sulphur poisoning, which is essential from the point of view of the necessary quality of the raw products used in the process. Considering the high activity of transition metal borides in hydrogenation reactions and their resistance to sulfur, the results of studies on the hydrotreating activity of NiB/SiO_2 catalyst in model reactions of hydrodenitrogenation (HDN) of carbazole alone and with hydrodesulphurization (HDS) of 4.6-DMDBT were presented. Their hydrogenation activity necessary during deep hydrotreating process.

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Cuprospinel as oxygen carrier for solid fuel combustion

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Keywords: cuprospinel, TGA analysis, solid fuel combustion

Cuprospinel ($CuFe_2O_4$) due to its relatively high oxygen transport capacity and capability to release gaseous oxygen in elevated temperatures (above 700 °C) in an anaerobic environment, is a promising material for oxygen carrier in the chemical looping combustion process (CLC). CLC is a low-emissive combustion technology that has the potential to be applied to the combustion of both gaseous and solid fuels. In the CLC process, oxygen needed for combustion is supplied entirety via an oxygen carrier. This approach combines the advantages of oxyfuel combustion without the necessity of constructing dedicated oxygen generators. Combining CLC with an effective carbon capture unit has the potential to achieve more carbon-neutral combustion of fossil fuels. Furthermore, using biomass as a fuel can result in net negative carbon dioxide emissions.

In this study, cuprospinel was utilized as an oxygen carrier for the combustion of various fossil fuels (coals) and a renewable fuel (waste biomass). The combustion process was monitored by using a thermogravimetric analyzer coupled with a quadrupole mass spectrometer for online analysis of the gases produced during the combustion process.

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Enhancing ci engine performance with ionic liquid and graphene quantum dots

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The increasing global population, depleting fossil fuel reserves, and environmental concerns have driven governments worldwide to promote alternative energy sources for transportation. This study investigates the effects of incorporating Ionic Liquid (IL) and Graphene Quantum Dot (GQD) into diesel fuel on the performance and emission characteristics of a two-cylinder, four-stroke diesel engine. Experimental findings show that while Brake Power (BP) remains nearly constant, the blend results in an average increase of 12.83% in Brake Thermal Efficiency (BTE) and an 11.35% reduction in Brake Specific Fuel Consumption (BSFC), highlighting improved fuel efficiency. A comparative analysis of BTE for diesel and the diesel-IL-GQD blend across different loads, as depicted in Figure 1, further supports the observed enhancement in thermal efficiency.

Furthermore, Density Functional Theory (DFT), a widely employed computational method in chemical reaction studies [1,2], indicates increased reactivity of the fuel blend compared to conventional diesel, suggesting potential combustion advantages. A cost assessment reveals that while the blend is currently only marginally economical, future advancements in large-scale production and technological improvements could enhance its viability as a sustainable alternative fuel.

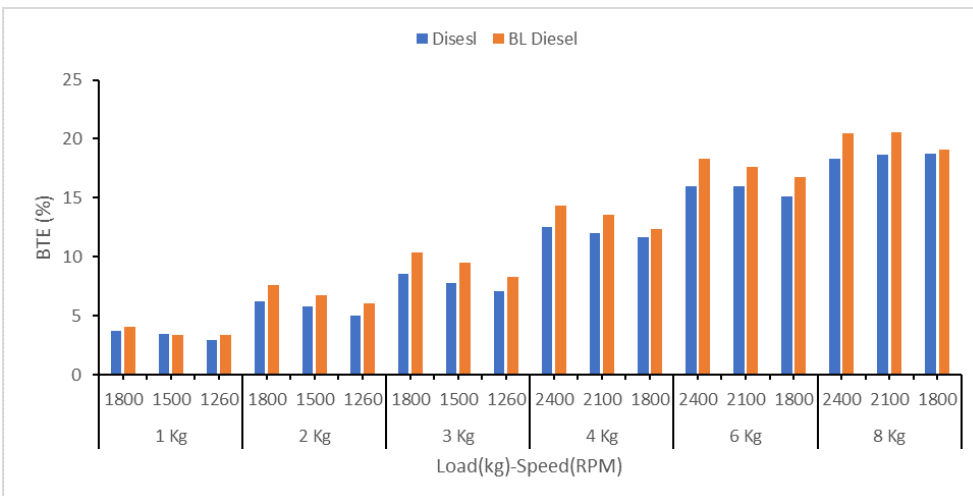

Figure 1: Comparison of the BTE for diesel and the diesel-IL blend at different loading of engine

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Thermogravimetric and calorimetric analysis of biocrude from pretreatment-enhanced hydrothermal liquefaction

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Keywords: protein extraction, acid hydrolysis, hydrothermal liquefaction, biocrude, TGA, HHV

The global shift toward carbon neutrality has increased the importance of organic waste valorization in sustainable energy systems. In Poland, one of the largest agri-food producers in the European Union, noticeable amounts of by-products such as brewer's spent grain (BSG) demonstrate high energy potential as feedstock to produce renewable energy carriers like biochar or biocrude. Hydrothermal liquefaction (HTL) is recognized as a effective thermochemical process for converting wet biomass into high-energy-density biocrude, surpassing notably the value of the raw material. Despite its application potential, the complex composition of lignocellulosic feedstocks often leads to biocrude with elevated oxygen and nitrogen contents, posing challenges for downstream upgrading and increasing overall operational costs [1,2]. Brewer's spent grain (BSG), a major by-product of the brewing industry, contains high protein and hemicellulose content, which consequently contributes to elevated nitrogen and oxygen heteroatom levels in biocrude. This prompts research into effective pretreatment strategies [3].

In this study, an integrated pretreatment strategy combining alkali protein extraction (PE) alongside diluted acid hydrolysis (AH), was applied to BSG prior to HTL. This approach aimed to reduce the hemicellulose and protein contents, thereby improving the quality of the resulting biocrude. Both thermogravimetric analysis (TGA) and calorimetric methods, together with elemental CHNS analysis, were employed to characterize the thermal stability, distillation potential, and energy content of the biocrude. Each pretreatment was conducted under specific conditions: (i) PE at 60 °C, 10 wt%, pH 12 for 120 min, and (ii) AH at 150 °C, 10 wt%, pH 2 for 180 min. The HTL process was carried out at 275°C for 15 minutes, using a 10 wt% concentration of dry biomass and a 1:1 water–ethanol solvent mixture. As a result, a liquid biocrude with a high heating value (HHV) in the range of 29.7–30.4 MJ/kg was obtained, which corresponds to an increase in the heating value of approximately 145% compared to the dry feedstock. The TGA analysis provided insights into distillation profiles, indicating that biocrudes derived from pretreated BSG exhibit a greater proportion of light distillable fractions (below 300 °C). Calorimetric measurements further confirmed elevated HHV values, attributed to a slightly increased carbon content and a lower sum of heteroatoms content, such as nitrogen and oxygen, in the biocrude matrix.

The findings highlight the crucial role of pretreatment in modifying biomass composition and improving energy efficiency of the entire process. Combining hydrothermal processing with the valorization of side products from protein and saccharide isolation opens new pathways in integrated biorefinery concepts. Such approaches reinforce the transition to sustainable bioenergy systems and promote the full utilization of agro-industrial residues within circular value chains.

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Thermal behaviour of hydrochars produced from apple pomace at different process temperatures: stability and value-added chemicals production

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Keywords: biomass, apple pomace, hydrothermal carbonization, hydrochar, pyrolysis, biochemicals

The food production industry produces large quantities of leftover by-products. Reasonable valorization of these streams could introduce new bioproducts into the market as eco-friendly substitutes for conventional products derived from fossil fuels. Therefore, new and innovative approaches are particularly sought. Poland, being a key provider of food products to the European Union market, represents a potentially abundant source of residuals and by-products, which should be harnessed effectively. The estimated annual production of fresh fruits and vegetables in Poland (e.g. apples, carrots, blackcurrants, and many more) has exceeded 10 million tons in recent years, with 3.9 million tons of apples supplied in 2023 [1]. Part of the fruits are consumed in fresh form, while the remaining are processed in a further way (juice, jams production), generating residual products such as pomaces or sludges. For instance, the share of estimated residual matter generated during apple processing can reach 25 – 30 wt.% of the input mass [2,3]. One of the most promising ways to utilise residual high-moisture matter, such as fruit pomace, is transformation by hydrothermal carbonisation (HTC), which has been intensively investigated over recent decades [4]. The produced hydrochar is a solid bioproduct with high energy density that can be used as an efficient energy carrier. It also provides several other applications, such as serving as a catalyst or fertilizer, and offers potential for chemical production *via* downstream processing. The presented work is in the field of valorization of food-producing waste through thermochemical processing. For this purpose, apple pomace as a high-moisture content by-product, was transformed into hydrochars through conversion under subcritical water conditions. The hydrochars were produced by hydrothermal processing over a wide range of processing temperatures, i.e. starting at 150°C and reaching up to 300°C. The main part of this contribution is the investigation of the thermal behaviour of the obtained hydrochars. The thermal behaviour of the hydrochars was investigated by microscale techniques, i.e. thermogravimetric analysis (TGA) and coupled pyrolysis–gas chromatography-mass spectrometry (Py-GC-MS). Thermogravimetric analysis indicated that the increase in HTC temperature enhanced the thermal stability of derived hydrochars and reduced the number of stages during thermal degradation. The study of volatiles released during pyrolysis showed a similar qualitative composition, although some quantitative variations were observed. The compounds released during pyrolysis constituted perspective chemicals with a high share of oxygen-containing compounds (e.g. ketones, furans, and aldehydes), which also could demonstrate application potential.

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Production of green diesel via oleic acid hydrodeoxygenation over carbon-supported nickel catalysts

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Keywords: hydrodeoxygenation, oleic acid, green diesel, nickel catalyst, carbon support

Several methods of biomass conversion to biofuels were developed to provide the competitiveness of biodiesel to petrodiesel. The main commercial route for obtaining biodiesel is upgrading lipid feedstock, such as edible or non-edible vegetable oils, animal fats and residual fats. They are a source of long-chain fatty acids or triglycerides, which can be transesterified with alcohols to produce fatty acid alkyl esters (FAAE) – the first generation biodiesel. A promising alternative to the ester-based biofuel is so-called 'green diesel', the product of hydrodeoxygenation (HDO) of lipid feedstock, a bio-component fully compatible with diesel. HDO is a method of producing the next-generation biodiesel, which seems to be superior to the first-generation fuel. The HDO process allows for a degradation of oxygen-rich fatty acids, which reduces the oxygen content, increases the C:H ratio and cetane number, and improves the overall green diesel quality. The most important advantages of green diesel are the high yield of the diesel-range biofuel, consisting mainly of C15-C18 hydrocarbons, and high cetane number, which can be attributed to elimination of the oxygen [1]. The HDO process occurs via three paths: decarboxylation (DCX), decarbonylation (DCN) and direct hydrodeoxygenation (direct-HDO). During the DCX and DCN paths, oxygen is completely removed in the form of CO_2 and CO, producing hydrocarbons with one less carbon atom in a molecule. In the direct-HDO path, oxygen is removed in the form of H_2O, and the hydrocarbons have the exact same number of carbon atoms as the starting molecule. The products of HDO process include hydrocarbons (C15-C18) and their unsaturated isomers, alcohols, aldehydes and unconverted fatty acids. The HDO process requires high hydrogen pressures (up to 250 bar) and moderate temperature (200-400 °C), and is performed in the presence of a catalyst [2, 3]. Most commonly used HDO catalysts include transition metals (Ni, Mo, Co) and noble metals (Pt, Pd, Ru) supported on various materials, among others silica, alumina and carbon supports [1-5]. One of the challenges of producing green diesel via HDO process is a proper selection and preparation of the catalytic system. In this work, the HDO process of oleic acid over Ni catalysts supported on mesoporous carbon materials is investigated. The reactions were conducted at 60 bar H_2 pressure and 320 °C in a varied contact times, using different Ni loadings (10, 25 and 40 wt%) in catalysts. The products were identified by Gas Chromatography (GC-FID), and the properties of the catalysts were characterized (BET, 2D-NLDFT, XRD, XRF). The conversion of oleic acid was from 70 to 100 % and varied with contact time and Ni content. The reaction paths were also discussed. To the best of our knowledge, a similar research has not been reported yet.

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Comparative analysis of diesel and waste cooking oil blends on engine performance and emissions using statistical and machine learning approaches

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Keywords: alternative fuels, waste cooking oil, diesel blends, engine emissions, particle number, Kruskal–Wallis test, neural networks, regression modelling

This study investigates the influence of different fuel types—pure diesel and its blends with 20% and 40% waste cooking oil (WCO)—on engine performance and emissions. The experimental campaign was conducted across a range of engine speeds, loads, and air–fuel ratios (Lambda), measuring brake thermal efficiency (BTE), brake specific fuel consumption (BSFC), and emissions including CO, CO_2, HC, NO, and particle number (PN). Statistical significance of the fuel type on each output variable was evaluated using the Kruskal–Wallis test, revealing notable differences, especially in CO and PN emissions. To further explore the complex relationships between engine operating conditions and outputs, mathematical models were developed using constrained regression and artificial neural networks. These models enabled the generation of contour plots, which provided insights into optimal operating parameters for each fuel type. Moreover, composite indicators were constructed to assess the overall environmental and energetic impact of each fuel blend. The study highlights the potential of WCO blends as partial diesel substitutes, demonstrating their trade-offs in efficiency and emission performance.

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T10: Geosciences and minerals

Past and present of thermal analysis in the geological survey of Hungary

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Keywords: earth sciences, history, phase analysis, minerals, DSC

The Geological Survey of Hungary has a historical role and experiences in the application of thermal analysis to solving geoscientific problems (e.g. genetics and crystallinity of montmorillonite and kaolinite in raw materials: bauxite, bentonite, kaolin) [1, 2]. Thermally active minerals were identified in bulk rock samples (powdered below 63 μm) for both qualitative and quantitative phase determination [3]. The first commercial simultaneous thermogravimetry and differential thermal analysis instrument the Derivatograph(-PC) [4], was used and strongly accompanied by X-ray diffraction and infrared spectroscopy in our institution in the last century. Currently thermal analyses at the Geological Survey of Hungary is carried out with a Netzsch STA 449 F5 Jupiter instrument which can simultaneously perform TGA and DSC measurements. The instrument is also equipped with an automatic sample charger (ASC). The crucibles are made from Al_2O_3, where 50 mg powder sample (<63 μm) is measured, and the temperature of the furnace is regulated by a linear heating program at a rate of 10°C/min until 1100°C. For the evaluation of the data, Proteus 8.0 software is used. We use thermal methods combined with X-ray diffraction, which is suitable for phase analysis, identification of minerals from wide range of geological samples. For this a Bruker D2 Phaser XRD powder diffractometer (CuKα radiation, 30kV, 10mA) in Bragg–Brentano geometry, in Theta/Theta vertical goniometer alignment is used. In addition for most samples infrared spectroscopy is applied as well. Attenuated total reflection Fourier transform infrared (ATR-FTIR) spectroscopy is a very sensitive non-destructive method to identify OH-bearing phases. The samples usually analysed by a Bruker Vertex 70 Fourier-transformation infrared (FTIR) spectrometer equipped with a Bruker Platinum diamond ATR cell and a MCT detector. The combination of these three techniques has a key role in phase analysis of geological samples e.g. final deposition of low- and intermediate-level radioactive waste (Püspökszilágyi, Üveghuta); mapping works for Radioactive Waste Treatment and Disposal Facility at Püspökszilágy; participation in making the research plan for the Boda Siltstone Formation – in the frame of the programme for the deposition of high level radioactive waste; detailed investigations of a sedimentary bentonite site (Sajóbábony) [5], complex research of sedimentary kaolinitic sandstone in Hungarian Paleogene Basin; understanding the water-rock-CO_2 system for long-term CO_2 geological storage, especially the presence of dawsonite and its stable H isotope determination [6]; and also these methods are significant for the short-term H_2 geological storage to follow the potential reaction in the H_2-water-rock system.

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Optimization of functional properties of clay raw materials using integrated thermal analysis methods

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Keywords: clay raw materials, thermal analysis, mineralogical characterization, sintering behavior, functional optimization

Clay is a widely used raw material in ceramics and construction, but it also holds great potential in environmental engineering, especially in waste management and sustainable material production. One of the key applications in this field is the use of clay to incorporate industrial and municipal waste into sintered materials, such as lightweight aggregates like expanded clay. By adding waste-derived components to the mineral composition of clays, it is possible to create high-performance materials while reducing environmental impact [1].

Thermal analysis plays a crucial role in understanding how different clay compositions, including those modified with waste materials, behave during processing. Techniques such as differential scanning calorimetry (DSC) and thermogravimetry (TG/DTG) help identify how both the clay and added waste decompose when heated, ensuring that the right temperatures and conditions are used during firing. Many industrial by-products, such as fly ash from coal power plants, sewage sludge, or metallurgical slag, contain useful compounds like silicates and oxides, which can enhance the sintering process and improve the final properties of the material. By carefully analysing phase transformations, it is possible to modify raw material compositions to achieve better strength, porosity, and thermal insulation properties.

Other methods, like laser flash analysis (LFA), provide information about the thermal conductivity of the final product, which is especially important for materials used in insulation or energy-efficient construction. Dilatometry (DIL) helps measure how much the material expands or shrinks during heating, ensuring that waste additives do not cause excessive deformation. Hot-stage microscopy (HSM) allows for direct observation of softening and melting processes, helping manufacturers fine-tune the composition and firing conditions of the clay.

Incorporating waste materials into clay-based products is an effective way to reduce industrial and municipal waste while creating valuable new materials. Expanded clay aggregates modified with waste components are lightweight, durable, and porous, making them ideal for use in lightweight concrete, filtration systems, and soil stabilization. Their porous structure helps them absorb pollutants, making them useful for cleaning water and protecting the environment.

By studying how clay materials behave at high temperatures, scientists and manufacturers can improve their composition and make production more efficient. This method also helps recycle waste into valuable products while using less energy. Thanks to these advancements, clay is becoming even more important in eco-friendly construction and environmental engineering, helping to create better and more sustainable solutions for modern industry.

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Physical characterisation of a porous precious play-of-colour opal

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Keywords: hydrous silica, opal-CT, TG, BET, DSC, FT-NIR

Precious opal displaying play-of-colour (POC) is a hydrous silica ($SiO_2.nH_2O$) which is found in two general morphological forms, an amorphous form, opal-A, and a paracrystalline form, opal-CT. Both forms are predominantly composed of silica with circa 1% aluminium (as network former), 0.5% alkali and alkali earths and typically 6 to 7 % water, although the water content can vary significantly and can range up to circa 20% [1,2].

The water contained in opal is present in both bound and molecular forms and can be characterised by a range of methods including thermal and spectroscopic methods [1]. The bound water is present as silanol at internal (pore and void) and external surfaces, as well as distributed through the silica network as broken linkages between SiO_4 tetrahedra. Molecular water is present in pores and voids and is also distributed in cages in the silica network. Typically, the molecular water is trapped in the opal as the pores anda voids are not interconnected nor exposed to the surface. However, certain specimens of precious opal displaying POC have interconnected pores which are exposed to the surface and can freely absorb or desorb water [2]. An example of this type of opal is the subject of this study.

The opal specimen under investigation was sourced from the Wollo region of Ethiopia and displays play of colour. As the opal is porous, water can be reversibly removed from the opal. To characterise the opal, a range of analytical techniques were applied. Gas adsorption, low temperature DSC and low temperature FT-NIR were applied to the characterisation of the pore structure resulting in an observed pore diameter in the range 2 to 6 nm consistent with previous observations [3]. TG and high temperature FT-NIR were carried out to investigate the removal of the water from the pores through multiple heating-cooling cycles. The removal of the water was found to be reversible up to 15 cycled between room temperature and 600°C. In addition, low temperature DSC was also carried out on heated treated opal to identify the temperature limits in which crystallisable water could be retained in the opal. The results of this paper are reported and used to help the understanding of the type of opal-CT which contains interconnected pores.

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T11: Heat transfer

Optimization of mixed convection heat transfer in hybrid nanofluid flow with heated fin structures in circular tubes for heat exchanger applications

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Keywords: mixed convection, heat transfer, hybrid nano fluid, circular tube, rotating fin, numerical computation

This study used a novel strategy of inserted fins along the circular cylinder to pretend laminar flow numerically. Cylinder is not fixed it is a rotating cylinder. Adding fins to the rotating cylinder with hybrid nanofluid aids the obvious goal of increasing the heat transfer progression's efficiency. These fins were supplementary in repeat sets, with the fin height rising with each set. The stirring fins and the outer walls are hot. The heat conduction is practical from the hot walls to water. The gravitational and electrical conductivity practical on the hybrid nanofluids. Using the ANSYS FLUENT tool, the finite volume method was used to do the 3D imitations. The numerical simulations show that the inner circular domain exposes some closed contours that stipulate the recirculating flow configurations motivated by rotating fins and the being of hybrid nanoparticles. The rotating fins yield deformation stress that aids in flow circulation and high velocity, and buoyancy forces also play an important role in propelling the flow with collective Grashof number values. The flow velocity is abetted by growing Grashof number values, with the maximum value occurring close to the rotating fins' surface. Added to it reveals that an increasing velocity flow profile with increased nanoparticle concentration inside the rotating fins region. This is transported on by the nanofluid's altered viscosity and improved thermal conductivity. Higher nanoparticle concentrations refine heat flux, which lowers flow confrontation and increases flow near rotating fins. The presence of nanoparticles facilitates more intense flow by indorsing shear stresses and boundary layer stability.

Experimental assessment on the thermal and moisture migration of sand-based backfill materials combined with fly ash

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Keywords: sand, backfill materials, fly ash, thermophysical properties, thermal and moisture migration,water retention

To ensure cleanliness and environmental protection while alleviating the increasing pressure of building heating, ground source heat pump (GSHP) technology, which utilizes shallow geothermal energy that is helpful for net-zero emission reduction targets in place, has attracted wide attention due to the stable temperature of the soil. Improving the flow and heat transfer performance of ground heat exchangers (GHEs), would effectively improve the overall thermal economy of GSHP system. Thermal and moisture migration in backfill materials have critical impact on the performance of GHEs.The thermo-physical properties of the backfill materials play a significant role in the thermal performance of ground heat exchangers (GHEs). The thermophysical properties and thermal and moisture migration characteristics in sand-based backfill materials were evaluated in terms of fly ash additive. The average thermal conductivity of sand/10% fly ash mixture between moisture contents of 0~20% lifted by about 34% in comparison with that of parent sand, while the average specific heat capacity dropped by about 10%. The average apparent thermal diffusivity of the sand/10% fly ash blend grew by about 64% compared with the parent sand, while that of the sand/5% fly ash blend rose by about 28%. The moisture migration degree for the sand/5% fly ash blend and the sand/10% fly ash blend diminished by about 66% and 79%, respectively, compared to the parent sand. The fly ash additive promoted the thermal diffusion of sand-based backfill materials, due to its high-water retention and thermophysical properties. Therefore, the additives with both high thermal conductivity and water retention would be feasible options for prompting the thermal performance of the GHEs. And fly ash could be recommended as an excellent additive for sand-based backfill materials in GHEs. The data can provide some reference for the design and operation of the GHEs.

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Literature review on coatings and coating processes for optimizing heat dissipation in brake systems

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Keywords: coating, heat dissipation, heat transfer

The efficiency, lifespan, and operational stability of brake systems are significantly influenced by the coatings and coating processes applied to their components. This study provides a comprehensive literature review on various coating technologies, with a particular focus on those applicable to brake units. Based on the reviewed literature, different coating materials and processes are categorized and compared, highlighting their thermal conductivity, wear resistance, corrosion resistance, and mechanical properties.

The review presents the most widely used coating techniques, including thermal spraying, physical and chemical vapor deposition, as well as electrochemical and other specialized coating processes. The analysis explores the advantages and limitations of each technology in the operational environment of brake systems and examines how they contribute to optimizing heat dissipation. Furthermore, innovative coating solutions from various industries are investigated for their potential adaptability to brake technology advancements.

The primary objective of this literature review is to provide a comprehensive overview of the development trends and application possibilities of coating technologies, thereby facilitating the design of more efficient and durable brake systems. The findings may contribute to improving thermal performance, extending system lifespan, and developing more sustainable solutions, which could be beneficial for both transportation and industrial applications in the long run.

Optimization of Functional Filler Application and Regulation of Thermal Release Characteristics in Reconstituted Tobacco

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Keywords: Cellulose nanofibrils (CNF), thermally conductive reinforcements, thermally conductive composite materials, heat conduction, heat-activated release, hexagonal boron nitride (BN)

This study addresses the critical challenges in optimizing the release efficiency and stabilizing the regulation of fundamental components in heated tobacco products (HTPs) aerosol. Focusing on the heat-mass transfer mechanisms within the porous media of reconstituted tobacco (RT), the optimization of functional filler application and thermal release regulation were systematically investigated. Through multiphase flow characterization and heat-mass transfer theory in porous media, cellulose nanofiber (CNF) was introduced as an activating material for the functional filler boron nitride (BN), achieving effective exfoliation of BN lamellae and homogeneous dispersion. This strategy significantly enhanced the interfacial bonding between filler and matrix, thereby improving the thermal activity and response consistency of RT during heat transfer processes. The research established quantitative relationships between key structural indicators and thermal release characteristics, enabling three critical advancements: 1) optimized internal structural morphology design, 2) effective functional filler application, and 3) directional regulation of thermal conversion properties. These findings provide both technical solutions and theoretical foundations for precise control of HTPs aerosol release.

Human-induced airflow and particle transport in isolation wards: CFD assessment of ventilation effectiveness

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Keywords: Human-induced airflow, thermal microenvironment, computational fluid dynamics, air curtain, localized exhaust, indoor air quality

This study investigates the transient thermal effects of human movement on airflow and particle transport in burn isolation wards, aiming to evaluate the effectiveness of different ventilation strategies using Computational Fluid Dynamics (CFD). A validated CFD model simulates airflow and particle dispersion within a single-bedded isolation ward, incorporating a walking thermal manikin to replicate human-induced thermal plumes and motion-driven airflow disturbances. The baseline ventilation system consists of ceiling-mounted diffusers and local exhaust ventilation operating at 6 ACH. Four additional cases were simulated, incorporating variations such as increased air changes per hour (ACH), air curtain systems, and localised exhausts. The results reveal that increasing ACH alone (Case 1) offered only marginal improvement in reducing particle settlement. In contrast, Case 2 and Case 3, which utilised double air curtains with and without local exhaust, significantly reduced particle settlement by 68.6% and an additional 37.5%, respectively. Most notably, Case 4 (a single air curtain paired with localised exhaust) successfully eliminated particle settlement on the patient and bed surfaces within 10 seconds. These findings confirm that airflow disturbances caused by human movement can be effectively managed with strategically designed ventilation systems, thereby enhancing infection control and indoor air quality in healthcare environments.

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Research on the application of multidimensional thermal analysis technology in stock tobacco raw material usage recommendation and cigarette manufacturing quality tracking

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Keywords: multidimensional thermal analysis, stock tobacco raw material, cigarette manufacturing quality

For a long time, the recommendation for the use of tobacco raw materials in stock and the quality tracking of cigarette manufacturing processes have mainly relied on sensory evaluation opinions, and the evaluation results of sensory quality mainly depend on people's subjective experience of smoke, which has certain limitations. Smoke is a product of the heating process (pyrolysis, combustion) of tobacco, and thermal analysis techniques can be used to quantitatively characterize the release process of smoke and some chemical components of tobacco. This work intends to use a thermogravimetric analyzer to detect the smoke release process of stock tobacco raw materials or manufacture process samples (within or between batches), and at the same time use chromatographic analysis technology to detect tobacco volatile components. Based on the above detection results, multidimensional data analysis algorithms such as weighted or prioritized methods will be used to quantitatively describe and analyze the characteristics of tobacco raw materials or the quality fluctuations of cigarette manufacturing processes. The evaluation principle for the similarity of stock tobacco raw material characteristics or stability of cigarette manufacturing process quality is to try to find the minimal data differences between samples, which will provide a strong basis for recommending the use of stock tobacco raw materials and tracking the quality of cigarette manufacturing processes.

Heat and fluid flow investigation of synthetic jet impingement in electronic cooling

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Keywords: synthetic jets, mean heat transfer coefficient, parabolic cavity, conical cavities, fluidic efficiency

Electronic devices are moving towards a new level of development stage with the rapid miniaturization leading to extremely high heat accumulation. There is a higher demand for thermal management technology, especially in data centres. The growth of industries such as aviation has also exacerbated carbon emissions. As a consequence there is need for development of more effective heat dissipation techniques keeping the carbon footprints to a permissible level. Synthetic jet actuators (SJA) are among the most promising approaches to improve cooling performance although many other heat removal methods have been implemented over the past few decades. Synthetic jets are generated by the interactions of a train of vortices periodically drawn into and ejected from a cavity through an orifice. A typical synthetic jet actuator consists of an enclosed cavity with one or more openings (orifice or slot) on one side. The other face has a diaphragm for actuation. The oscillatory motion of the diaphragm leads to alternate suction and ejection of the fluid between the cavity and the cross-stream. During the suction stroke, the opening acts as a sink and entrains the near wall low momentum fluid into the cavity while during the expulsion stroke, a fluid jet accompanied by a train of vortices is formed. There is net momentum injection into the cross-stream without any additional mass addition. The present study involves investigation of two cavity shapes namely conical and parabolic of the SJA with respect to a cylindrical cavity. Synthetic jets produced from these cavities are made to impinge on a heated plate. The actuation frequency range of the SJA is varied within 5–60 Hz. The synthetic jet's velocity gradually drops in various proportions and for given actuation frequency the peak velocity in case of parabolic and conical cavity synthetic jet actuators are found to be 23% and 4.5% respectively higher producing more fluctuations and mixing than that of a cylindrical cavity. Fluidic efficiency follows a similar pattern and affects the mean heat transfer cooling rate during the impingement of the synthetic jet with heated plate.

Digital twin-enabled ventilation control for enhanced thermal comfort and sustainability in smart buildings: a review

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Keywords: indoor air quality, digital twin, neural network, sustainable energy, smart building

Thermal comfort is a cornerstone of occupant well-being in indoor environment, where ventilation systems regulate indoor temperature, humidity, and airflow distribution to maintain optimal conditions. However, conventional ventilation systems are highly energy-intensive, conflicting with global sustainability goals. The integration of IoT and digital twin technologies offers a transformative approach to balance occupant-centric thermal comfort with sustainability [1]. This review explores how IoT-enabled sensor networks and digital twins coordinate to create adaptive ventilation systems that respond in real time to spatial and temporal variations in thermal demands. Digital twins leverage Building Information Modelling (BIM), IoT sensor networks, computational fluid dynamics (CFD), and machine learning (e.g., GRU models for IAQ forecasting) to create dynamic virtual replicas of buildings [2]. By integrating real-time IoT data with predictive models, adaptive strategies like demand-controlled ventilation (DCV) [3] and model predictive control (MPC) [4] adjust airflow rates, cooling and heating cycles, and air distribution to align with occupant needs while minimizing energy consumption. The paper outlines a framework for developing digital twins focused on thermal comfort, emphasizing IoT-BIM interoperability, CFD-driven airflow optimization, and occupant feedback loops. Despite their potential, challenges such as multi-domain system integration, data accuracy, computational complexity, and scalability in heritage or heterogeneous environments limit adoption will be discussed. Future research must prioritize interoperability between digital twin platforms, AI-driven real-time decision-making, and scalable solutions for diverse building typologies. By addressing these gaps, digital twins can revolutionize smart building ventilation, advancing sustainability, resilience, and occupant-centric design while minimizing energy footprints. This review underscores the transformative potential of digital twins and outlines pathways to overcome existing barriers for broader implementation.

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Simulation-based assessment of solar still efficiency for freshwater production in the Aral Sea region

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Keywords: solar still, thermal desalination, Aral Sea region, heat transfer model, energy efficiency

This study presents a simulation-based assessment of the efficiency of single-slope solar stills for freshwater production in key settlements surrounding the Aral Sea, including Kulandy, Aral, and Uzynkair in Kazakhstan, as well as Taylakdzhegen and Moynaq in Uzbekistan. A mathematical model grounded in heat balance equations and solved using the Fourth Order Runge–Kutta method was employed to simulate the distillation process under the distinct climatic conditions characteristic of the Aral Sea basin. The results underscore the critical influence of geographic location, solar radiation, and ambient temperature on the performance of solar stills in this semi-arid, post-desiccation environment. Particular attention was given to the optimization of system parameters, such as basin water depth and insulation thickness, to adapt to local meteorological conditions. The findings suggest that solar stills offer a viable and sustainable solution for decentralized freshwater generation in remote and water-scarce communities of the Aral region. This study contributes to the growing body of research on solar desalination technologies adapted to continental climates and provides a foundation for future work involving hybrid renewable systems in environmentally stressed areas.

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Research on dynamic changes of moisture content and temperature in tobacco shreds during fixed-bed convective drying and Numerical simulation

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Keywords: fixed-bed, convective drying, heat-mass transfer, tobacco lamina shreds, numerical simulation

Drying is a critical process in cigarette manufacturing technology, inherently involving simultaneous heat and mass transfer. Fixed-bed drying, a typical convective heat transfer method, efficiently removes moisture through the interaction between hot air and material. This study investigates the dynamic evolution of moisture content and surface temperature of cut tobacco during convective drying using a fixed-bed drying apparatus. A heat and mass transfer kinetics model is developed based on lumped heat transfer theory, the assumption of free water inside tobacco shreds, and instantaneous vapor-liquid equilibrium. The results show that numerical simulations are highly consistent with experimental data. Accurately depicting heat and moisture migration under different drying temperatures (110-120℃). The model reveals that higher temperatures accelerate moisture evaporation, rapidly reducing moisture content and increasing surface temperature. But lower temperatures slow down drying. It also demonstrates the coupled heat-moisture transfer mechanism and precisely predicts real-time temperature-moisture responses. Sensitivity analysis quantitatively demonstrates the drying rate's strong dependence on air temperature. The results offer theoretical basis and model support for optimizing tobacco drying processes.

T12: Inorganic materials

Artificial intelligence-based prediction of outlet air and water temperatures in heat exchangers under sudden variations of input parameters

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Keywords: heat transfer prediction, compact heat exchangers, artificial neural networks, forecasting, modelling

This study presents a dynamic neural network model for simultaneous prediction of air and water outlet temperatures in heat exchanger systems under transient operational conditions. The framework integrates time-dependent inputs (flow rates, inlet temperatures, abrupt load variations) with geometric identifiers (fin density, tube configuration, surface area ratios) to forecast thermal performance across two distinct heat exchanger architectures. Artificial neural networks (ANNs) were trained on high-resolution experimental datasets capturing step changes, flow reversals, and stochastic disturbances. Prediction accuracy was quantified via the Theil coefficient and mean absolute error (MAE < 1.8 K), with a focus on response lag and error propagation during rapid transients (e.g., 20–80% load shifts within 10 s). The model demonstrated superior robustness compared to steady-state correlations, maintaining <4% MAPE even during nonlinear thermal inertia effects. Sensitivity analysis revealed that tube-side flow instability degrades water temperature predictions more severely than air-side perturbations. This data-driven approach enables predictive control of coupled heat exchangers, mitigates overshoot risks in transient-heavy applications, and provides insights into failure modes induced by extreme operational volatility

The impact of biocatalyst modification on the efficiency of silica recovery from plant waste

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Keywords: nanosilica, biotransformation, Trichoderma

Nanosilica is an important inorganic material widely used in various industries. The standard chemical production of silica nanomaterials is costly and requires extreme conditions of temperature, pressure, and pH, so it is harmful to the environment. In contrast, the process of biogenic silica formation by living organisms, including plants, occurs under physiological conditions. The presence of silicon in the form of SiO_2 in rice (*Oryza sativa*) was first described in 1938. Interestingly, the highest silica content in rice is found in its husk, ranging from 9% to 12%. According to FAO data, global rice production in 2023 is estimated at approximately 509 million tons [2]. Such large-scale production generates huge amounts of rice husk waste, which is difficult to dispose of. Previously published research indicates that the amorphous biogenic silica naturally deposited in rice husks can be transformed into valuable crystalline nanoparticles with industrial applications [1].

This study investigates the potential use of *Trichoderma harzianum* fungi as a biocatalyst in the silica recovery process and how different biocatalyst preparation methods affect the efficiency of this process. Six process variants were analysed to compare the effectiveness of biocatalyst modifications.

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2. FAO RICE MARKET MONITOR

The importance of the thermal analysis method in studying the formation of calcium hydroxyapatite and malachite green composite

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Keywords: calcium hydroxyapatite, malachite green, composite, formation

The development of new bioactive antibacterial calcium phosphate materials is still a very acute problem of modern science and technology [1]. Recently, it has been observed that hybrid organic-inorganic composites composed of functional antibacterial reagent and inorganic phosphates are promising tools against caries and periodontitis [2]. Promising antibacterial new bioceramic materials would be also those that would be effective in bone regeneration. It was also demonstrated in previous work, that the phosphogypsum waste could be successfully used as precursor for the synthesis of high quality bioceramic calcium hydroxyapatite [3].

In this study, using synthetic calcium hydroxyapatite ($Ca_{10}(PO_4)_6(OH)_2$; CHA) and functional dye malachite green (triarylmethane dye, $[C_6H_5C(C_6H_4N(CH_3)_2)_2]Cl$, MG), a new generation of bioceramic composites have been developed. Waste phosphogypsum, disodium hydrogen phosphate (Na_2HPO_4), sodium dihydrogen phosphate (NaH_2PO_4) and malachite green were used as starting materials for the fabrication of composite of calcium hydroxyapatite and malachite green *via* a dissolution-precipitation reaction. The CHA-MG composites having various concentrations of MG have been synthesized.

The prepared samples were characterized by powder X-ray diffraction (XRD) using a Rigaku MiniFlex II diffractometer with Cu Kα radiation (λ = 1.541838 Å). Fourier transform infrared spectroscopy (FT-IR) was performed using an Alpha spectrometer (Bruker, Inc., Germany) in the wavenumber range from 4000 to 450 cm^{-1}, with a resolution of 4 cm^{-1}. The product morphology was analyzed using field-emission scanning electron microscopy (SEM, SU-70, Hitachi, Tokyo, Japan). Chromatographic measurements were performed on an Agilent 1290 Infinity II LC system (Agilent, Waldbronn, Germany) equipped with a ternary pump, thermostatted column compartment, photodiode array detector and autosampler. Thermal analysis of the composite sample was examined by thermogravimetric analysis and differential scanning calorimetry (TG-DSC) using a Perkin Elmer STA 6000 Simultaneous Thermal Analyzer. Approximately 10 mg of dried sample was heated from 25 °C to 900 °C at a heating rate of 10 °C/min in the flowing air atmosphere (20 mL/min).

The results of the TG-DSC measurements confirmed that the formation of CHA-MG composites depends on the synthesis conditions. TG-DSC analysis clearly showed that investigated organic-inorganic composite samples are composed of several phases. The results obtained demonstrated that TG-DSC analysis is indispensable tool in order to learn some special technological features of formation new bioceramic composites. Finally, the proposed new antibacterial composites for bone regeneration with enhanced antibacterial properties are very original and ambitious for future applications in biomedicine.

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Study on thermal behavior of mixtures of ammonium nitrate and various iron chelates

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Keywords: ammonium nitrate, iron chelates, thermal analysis, safety assessment

The integration of micronutrient additives into ammonium nitrate (AN)-based fertilizers has raised questions regarding the impact of such additives on thermal stability [1-5]. This study investigates the thermal behavior of AN mixtures containing various iron chelates commonly used in agricultural applications. The following compounds were examined: ethylenediaminetetraacetic acid (EDTA), iminodisuccinic acid (IDHA), diethylenetriaminepentaacetic acid (DTPA), N-(2-hydroxybenzyl)ethylenediamine-N,N',N'-triacetic acid (HBED), ethylenediamine-N,N′-bis(2-hydroxyphenylacetic acid) (EDDHA), and ethylenediamine-N,N′-di[(2-hydroxy-5-sulfophenyl)acetic acid] (EDDHSA). Thermal analysis was performed using TG-DTA-DTG methods, with chelate content adjusted to represent up to 0.5 wt.% Fe.

The aim of the study was to assess the thermal compatibility of these systems under conditions relevant to fertilizer production and storage. Results demonstrate that the presence of iron chelates generally reduces the thermal stability of AN and advances the onset of exothermic decomposition. Additional comparisons were made with previously analyzed mixtures of AN and inorganic iron salts (nitrates and sulfates), as well as chelates of copper, manganese, and zinc based on EDTA and IDHA.

The findings highlight the potential hazards associated with enriching AN-based fertilizers with certain iron chelates, particularly under conditions conducive to thermal runaway. These insights may inform future guidelines for the formulation of micronutrient-enriched fertilizers containing high concentrations of AN.

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New data on crystal phases in the system $MgSO_4$–$OC(NH_2)_2$–H_2O

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Keywords: urea complexes, magnesium sulfate, crystal structure, thermal behaviour

Urea complexes of magnesium sulfate have been intensively studied since the beginning of the last century due to their application in many areas of life, including agricultural chemistry, pharmacy, medicine, etc. Some of the results in this field refers to studies of the $MgSO_4$–$OC(NH_2)_2$–H_2O system and/or relationship between synthesis conditions and stoichiometry of the obtained $MgSO_4 \cdot nOC(NH_2)_2 \cdot mH_2O$ phases. Others relate to optimization of the processes for preparation of products for the agrochemical industry, which include urea and magnesium sulfate composites. Among the results obtained, the following ones are relevant to our study [1]. Both the reactants and final products of the system are temperature sensitive and, even at the same ratio of starting reactants, a small difference in the temperature range leads to the formation of stoichiometrically different phases. For instance, when a solution of $MgSO_4$ and $OC(NH_2)_2$ in molar ratio 1:1 is evaporated at 25 °C the product is $MgSO_4 \cdot OC(NH_2)_2 \cdot 3H_2O$, whereas an evaporation at 30 °C or 35 °C leads to the formation of $MgSO_4 \cdot OC(NH_2)_2 \cdot 2H_2O$. Diversity of magnesium sulfate sources and their pre-activation treatment are allowable, as presented in the patents WO2013/098367, US 2014/0360239 A1, and US 2016/0046534 A1. The authors describe conditions for obtaining mixtures of some of the above mentioned compounds using $MgSO_4$ or $MgSO_4 \cdot 7H_2O$ as magnesium sources and reactivation temperatures varying in the range 40–95 °C. The main preparation methods are synthesis from solution and mechanoactivation, while US 2016/0046534 A1 reports procedures combining the features of both methods. All the compounds reported above have been obtained from solution, whereas only $MgSO_4 \cdot 6OC(NH_2)_2 \cdot 0.5H_2O$ has been obtained by mechanoactivation as a pure end product. The solvent type plays a key role for the run products, thus $MgSO_4 \cdot OC(NH_2)_2 \cdot 2H_2O$, $MgSO_4 \cdot OC(NH_2)_2 \cdot 3H_2O$, $MgSO_4 \cdot 4OC(NH_2)_2 \cdot H_2O$ and $MgSO_4 \cdot 6OC(NH_2)_2 \cdot 0.5H_2O$ have previously been obtained by evaporation from water solutions. In other cases, a methanol solution has been used as a medium e.g., $MgSO_4 \cdot 5OC(NH_2)_2 \cdot 2H_2O$ and $MgSO_4 \cdot 6OC(NH_2)_2 \cdot 2H_2O$. The aim of our study is to add new knowledge about the trends and consistencies in the preparation procedures of $MgSO_4 \cdot nOC(NH_2)_2 \cdot mH_2O$ phases. A set of analytical methods was used to characterize their structure, thermal and spectroscopic properties. The conditions for preparation of pure $MgSO_4 \cdot OC(NH_2)_2 \cdot 2H_2O$, $MgSO_4 \cdot OC(NH_2)_2 \cdot 3H_2O$, $MgSO_4 \cdot 4OC(NH_2)_2 \cdot H_2O$ and $MgSO_4 \cdot 6OC(NH_2)_2 \cdot 0.5H_2O$ were specified (evaporation from dilute aqueous solutions) and of pure $MgSO_4 \cdot OC(NH_2)_2 \cdot 3H_2O$ and $MgSO_4 \cdot 6OC(NH_2)_2 \cdot 0.5H_2O$ (upon mixing MgSO4·nH2O and urea in appropriate ratios and by applying mechanoactivation). The crystal structures of $MgSO_4 \cdot OC(NH_2)_2 \cdot 2H_2O$, $MgSO_4 \cdot OC(NH_2)_2 \cdot 3H_2O$ were determined and their features were compared with previously published structures of $MgSO_4 \cdot 4OC(NH_2)_2 \cdot H_2O$ and $MgSO_4 \cdot 6OC(NH_2)_2 \cdot 0.5H_2O$. Certain spectroscopic characteristics (IR and Raman) of the

studied compounds were reported for the first time and the results were analyzed with respect to the specific properties of the chemical composition. Thermal analysis establishes a direct relationship between the thermal stability of the studied compounds, as well as the decomposition temperature of urea and the $OC(NH_2)_2$:H_2O ratio in the octahedral environment of the magnesium ion in the structures of the respective compound. Based on the thermal analyses data, it could be concluded that the number of water molecules in the crystal structure is of particular importance for their thermal behavior and stability. It is evident that as the water content of the compound decreases, both melting point and urea decomposition temperature increase. The substitution of urea for water also plays a role in the structure stabilization, with the most stable structure being the one in which the magnesium surrounding involves solely urea moieties. Such a type of thermal stability trend has also been observed for other crystal hydrate adducts of urea.

Acknowledgments
The authors thanks to the Bulgarian National Science Fund (grant agreement КП-06-Н64/4, 15.12.2022) for the financial support.

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Crystal phases in the system $MgCl_2$–$OC(NH_2)_2$–H_2O: synthesis and their thermal behaviour

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Keywords: urea complexes, magnesium chloride, crystal structure, thermal behaviour

Magnesium chloride forms hydrates with different numbers of water molecules in the crystal structure. So far, crystal chemical data have been reported for the compounds $MgCl_2$-nH_2O with n = 1, 2, 4, 6, 8, 9, 10, 11, 12, where the number of water molecules depends on the temperature, pressure and amount of water in the system. The hexahydrate ($MgCl_2$•$6H_2O$), the mineral bischofite, is the most common in nature. The physicochemical properties, processes, dehydration and decomposition of magnesium chloride hydrates have been intensively studied in connection with the application of these compounds in many areas of industry and medicine. In comparison, urea complexes of magnesium chloride are poorly studied. Knowledge of the compounds of this system and their physicochemical characteristics is important because the ability of magnesium chloride to form complexes with urea find various applications: magnesium chloride is used to purify waters rich in urea, mixtures of magnesium chloride and urea are used in the food industry (extracting and stabilizing agents, agronomic biofortification of cereal and legume waste, etc.) and in recent years as part of energy storage systems and aqueous rechargeable magnesium batteries. [1,2,3,4]. The aim of this study is to add new knowledge about the crystal phases in the system $MgCl_2$•$nOC(NH_2)$•mH_2O and their thermal behaviour. The conditions for obtaining Cl_2•$OC(NH_2)_2$•$4H_2O$, $MgCl_2$•$4OC(NH_2)_2$•$2H_2O$, $MgCl_2$•$6OC(NH_2)_2$, $MgCl_2$•$10OC(NH_2)_2$ were specified. The crystal structures of $MgCl_2$•$OC(NH_2)_2$•$4H_2O$ and $MgCl_2$•$6OC(NH_2)_2$ were solved for first time while the ones of the $MgCl_2$•$4OC(NH_2)_2$•$2H_2O$, $MgCl_2$•$10OC(NH_2)_2$ were reported earlier [5] The thermal behaviour of the four studied phases was investigated in the temperature range from room temperature to 600˚C using the DSC-TG method. In-situ powder diffraction analyses were applied in order to clarify the structural transformations upon heating. Research reveal a phase-specific thermal behaviour. Hydrate phases evolve water molecules differentially, forming intermediate crystalline phases. After 170˚C, the release of volatiles from urea begins. X-ray diffraction data show that after this temperature crystalline phases are only available from the decomposition of $MgCl_2$•$OC(NH_2)_2$•$4H_2O$. The two anhydrous phases have a similar behaviour, the unit cell shrinks upon heating and, as a result of the urea decomposition, the phases undergo amorphization.

Acknowledgments
The authors thanks to the Bulgarian National Science Fund (grant agreement КП-06-Н64/4, 15.12.2022) for the financial support.

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Application of thermoanalytical methods in the study of nir pigments based on doped $CaSnO_3$ perovskites

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Keywords: inorganic pigment, stannate, perovskite

The heating of buildings and other surfaces caused by exposure to sunlight represents a significant issue, placing a financial burden on households and companies worldwide. This heating is primarily caused by infrared radiation, which accounts for approximately 49 % of the solar radiation spectrum [1]. The negative effects of this phenomenon can be mitigated by applying special coatings to exposed surfaces. Such coatings often contain colour pigments with a reflectance of more than 20 %, known as cool pigments [2].

In addition to classic cooling pigments such as TiO_2 or ZnO [3], which are typically white, there are also coloured pigments with cooling properties, including $BiVO_4$, $CoAl_2O_4$ and $BiFeO_3$ [4]. The design of pigments that combine high reflectivity, attractive colour properties, excellent durability, and environmental friendliness remains an ongoing challenge for researchers worldwide.

In this work, new $CaSn_{1-x}M_xO_3$ pigments (x = 0.1; 0.2; M = Mn, Fe, Co, Ni) were prepared using three different methods: dry mechanoactivation, wet mechanoactivation, and precipitation, followed by high temperature calcination. The temperature required for the formation of the perovskite phase and the incorporation of dopants into the $CaSnO_3$ structure was investigated by the DSC-TG methods.

The calcination products were then characterised by X-ray diffraction analysis (XRD), X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), UV-VIS-NIR spectroscopy. The particle size distribution of the powders was analysed by low angle laser light scattering method and the effect of dopants on the thermal stability of the powders was tested by heating microscopy.

The prepared perovskite pigments exhibited a colour range from dark grey to brown, light brown, and beige. The lowest calcination temperature of 950 °C was insufficient to complete the reaction, while higher temperatures resulted in the formation of a spinel phase in the samples. Single phase pigments, $CaSn_{0.9}Mn_{0.1}O_3$ and $CaSn_{0.9}Fe_{0.1}O_3$, were successfully obtained via dry mechanoactivation and precipitation calcinated at 1100 and 1200 °C. The NIR reflectance measurements confirmed that these pigments can be classified as cool pigments. The precipitation method produced pigments with higher colour chroma, and the narrowest particle size distribution compared to the other methods, making it the most promising approach for future pigment preparation.

Acknowledgments
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T13: Kinetics and catalysis

Measurement of reaction kinetics between Perovskite-based oxygen carrier and gaseous fuel

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Keywords: perovskites, CLC, TGA analysis, reaction kinetics

Perovskites represent a fascinating class of materials, characterized by their overall formula of ABO_3. Due to the wide range of options for modifying their chemical composition, perovskites have a broad range of potential applications. Some perovskites can form oxygen vacancies in a reaction of changes in temperature and partial pressure of the oxygen in the reaction environment, therefore, such materials are potential candidates for oxygen carriers in a chemical looping combustion process (CLC). In CLC process, the oxygen carrier provides all the oxygen required for the combustion, therefore, the further carbon capture process is more simplified in comparison to conventional combustion. However, a good material should meet certain criteria such as high oxygen transport capacity, reactivity toward selected fuels, and also ability to retain its properties during numerous reduction oxidation cycles. In this work, perovskite-based materials were evaluated as potential candidates for the combustion of gaseous fuels. Tests were conducted on a thermogravimetric analyser as a function of temperature and gas partial pressure after which the reaction kinetic parameters such as energy of activation and reaction order were calculated. Furthermore, the model of gas-solid state reaction was also determined.

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The kinetic study of the drying process of food industry waste

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Keywords: drying of food industry waste, mathematical modelling, effective moisture diffusivity, activation energy

Drying techniques have been applied to food industry waste with the aim of preserving active compounds, reducing moisture to prevent mold formation, and optimizing their use in various applications [1,2]. For instance, spent coffee grounds can be safely stored if their final moisture content is kept below 10%, thereby preventing microbial growth. To determine the most effective drying process for this purpose, Tun et al. compared solar drying with convective oven drying and open-air drying [3]. Similarly, Badaoui et al. utilized solar energy for drying apple and orange waste. Their findings indicate that solar drying serves as a crucial intermediate step in processing agri-food waste intended for reuse [4].

In this study, the drying process of spent coffee grounds and apple puree was evaluated using a Mettler Toledo HG63 halogen moisture analyzer. This device employs a halogen lamp to heat the sample, accelerating water evaporation and reducing analysis time compared to traditional methods. The sample masses subjected to drying in the analyzer were 22.769±1.056 g for spent coffee grounds and 47.539±0.194 g for apple puree. The samples were evenly distributed on the equipment tray to ensure a uniform layer height. The experimental determinations were carried out at temperatures of 70 ºC, 80 ºC, 90 ºC, and 105 ºC. Based on the experimental measurements, the material moisture ratios (MR) and drying rates (figure 1) were calculated and plotted as functions of time and moisture content, respectively. The analysis of the drying curves revealed that diffusion is the primary mechanism for moisture removal during drying. Several models from the literature describing the drying process of food products were tested, and it was found that, in general, the best results for drying spent coffee grounds and apple puree were obtained using a modified Henderson and Pabis model.

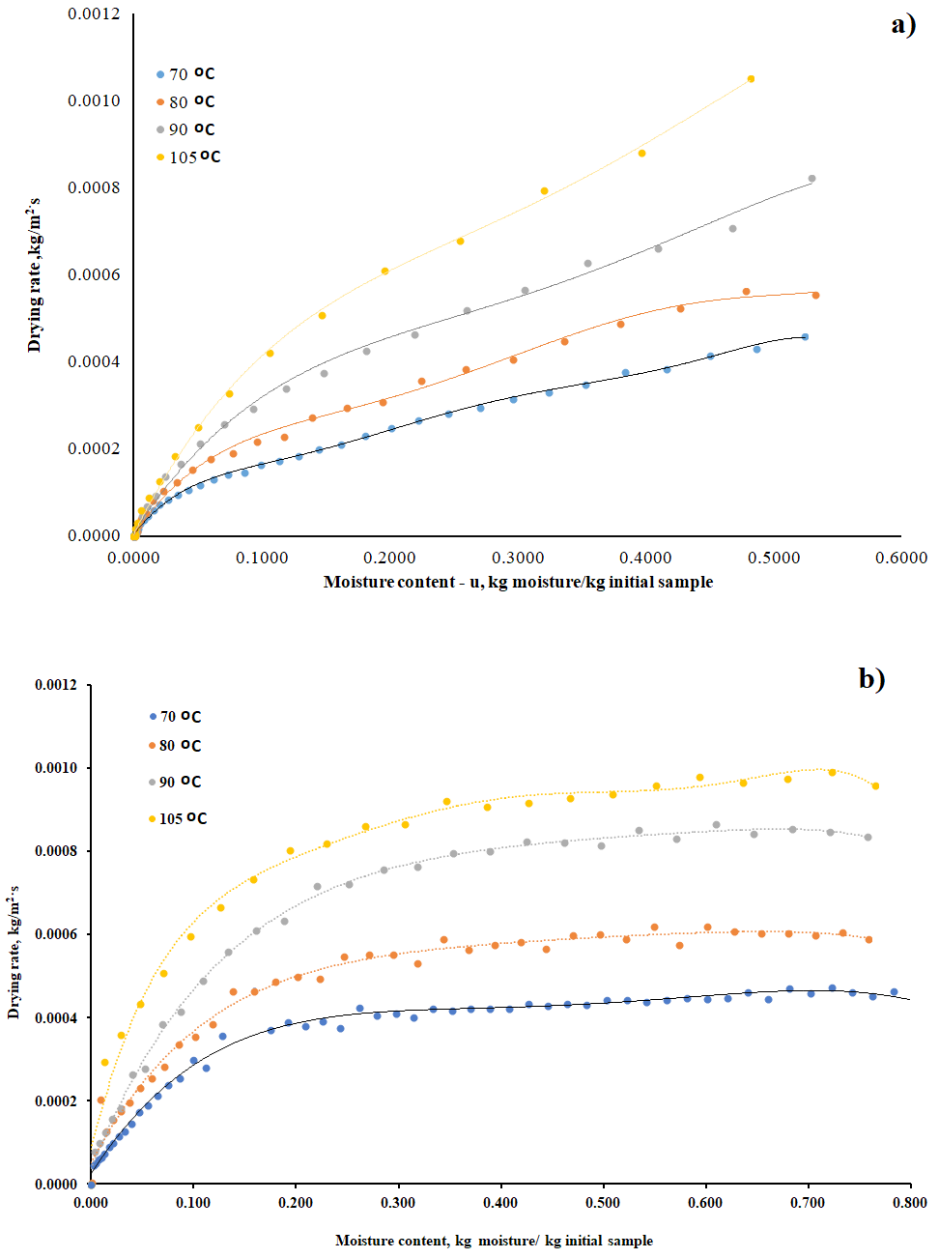

Figure 1. Variation of drying rate depending on humidity: a) spent coffee grounds and b) apple puree

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T14: Life sciences

Thermal stress and material fatigue in cargo parachutes

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Keywords: thermal stress, material fatigue, finite element method (FEM), numerical modelling

Cargo parachutes are subjected to significant thermal and mechanical stresses during the deployment phase due to the rapid deceleration and aerodynamic forces acting on the fabric structure. The sudden inflation of the canopy causes high velocity airflow, creating significant aerodynamic drag, while dynamic loading conditions lead to extensive mechanical deformation. These combined effects not only raise local temperatures within the material, but also cause long-term structural degradation, including material fiber weakening and potential thermal fatigue. This study investigates heat generation due to aerodynamic friction and mechanical deformation and evaluates its impact on fabric integrity. Finite element methods and digital modelling-based simulations are used to analyse the temperature distribution and thermal stresses.

This research aims to provide a better understanding of thermal effects on parachute materials by integrating advanced software techniques. The study is expected to contribute to the development of more durable and heat-resistant parachute fabrics, providing valuable information for aerospace and defence applications.

Entropy-driven approach to irreversibility management in ship engines

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Keywords: marine engine, bulk carrier, entropy, irreversibility, sustainability

The maritime industry, responsible for a substantial proportion (approximately 90%) of global freight transport, accounts for only a relatively minor proportion (approximately 3%) of total emissions. However, recent years have seen a notable shift in the approach taken by this sector to emissions. The formulation of ambitious emissions targets, coupled with the implementation of increasingly stringent regulations, has prompted the industry to pursue active strategies for the reduction of emissions. This proactive stance has prompted the development of studies that support solutions to fossil fuel consumption and alternative technologies. In particular, studies based on performance, such as those examining the diesel engine, which is the main consumer, have developed as pioneering studies. In the present era, internal combustion engine technologies are engines that are utilised in a multitude of sectors. In these engines, operational control strategies do not result in pollution caused by irreversibility, nor do they depend on environmental conditions. The thermal performance of engines is correlated with the generated power structure and directly affects the performance of the engines. In engines, this effect is actually a result of the entropy produced, which provides controllable results for thermodynamic design and operational processes. In this context, entropy-based evaluations of engines can be seen as an approach for the manageability of irreversibility. This study is based on a sectoral foresight approach. The impact of varying load distributions on the average engine power of bulk carrier ships was examined, with a particular focus on entropy-based considerations and environmental pollution. Furthermore, the potential for improvements in engine energy performance was evaluated. The average energy efficiency for engine powers, evaluated in six categories, was found to be 12.85%. Conversely, the improvement potential was 77.88%. These data indicate a high entropy of 564.67 kW/K. At the conclusion of the study, an evaluation of the entropy-based approach and its effects was presented.

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Determinants of carbon emissions: globalization, energy consumption and passenger transportation

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Keywords: ARDL, carbon emissions, energy consumption, environmental sustainability, globalization, passenger transportation, Türkiye

This study aims to analyze the determinants of carbon emissions in Türkiye by examining the impacts of globalization, energy consumption, and passenger transportation on environmental sustainability. The literature reveals that transportation and energy consumption significantly affect CO_2 emissions, with globalization potentially increasing emissions in developing countries. Using data from Türkiye for the period 1970-2016, the study employs Autoregressive Distributed Lag (ARDL) and Ordinary Least Squares (OLS) models to examine the short- and long-term effects of globalization, energy use, and passenger transportation on carbon emissions. The findings indicate that energy consumption has a notable impact on carbon emissions, while globalization indirectly increases emissions through rising energy demand. This study provides essential insights for policymakers aiming to develop sustainable environmental policies, highlighting the importance of reducing energy consumption and promoting eco-friendly transportation policies.

Preliminary studies of some pharmaceutical formulations with drugs from the anticoagulant class

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Keywords: anticoagulants, phenprocoumon, thermal analysis, thromboembolic disorders

Anticoagulants are essential agents for the prevention and treatment of thromboembolic disorders. Anticoagulant therapy is primarily aimed at preventing the formation of clots in blood vessels, which are the main cause of death in thromboembolic diseases. The paper presents the investigation by physico-chemical methods of the active substance Fenprocoumon, 3-(α-ethylbenzyl)-4-hydroxycoumarin. This study will complement our initiatives to develop superior therapies in this area. Phenprocoumon is rapidly absorbed after oral administration and has 100% oral bioavailability.

To successfully design a new pharmaceutical form, one of the main considerations in the early stages of the process is the compatibility study with excipients such as anhydrous lactose, talc, magnesium stearate, colloidal silicon dioxide, polyvinylpyrrolidone K30, starch, xylitol, mannitol, hydroxypropyl methyl cellulose. Binary mixtures were prepared by mortaring equal masses of phenprocoumon and each excipient in agate crucibles for 5 min. The solid samples were then sieved and transferred to sealed vials and stored at ambient conditions until analysis. The thermally induced interaction for the binary mixture between phenprocoumon and the excipients was studied using a TG/DTG/HF (see Fig. 1) and FTIR (see Fig. 2) analyses.

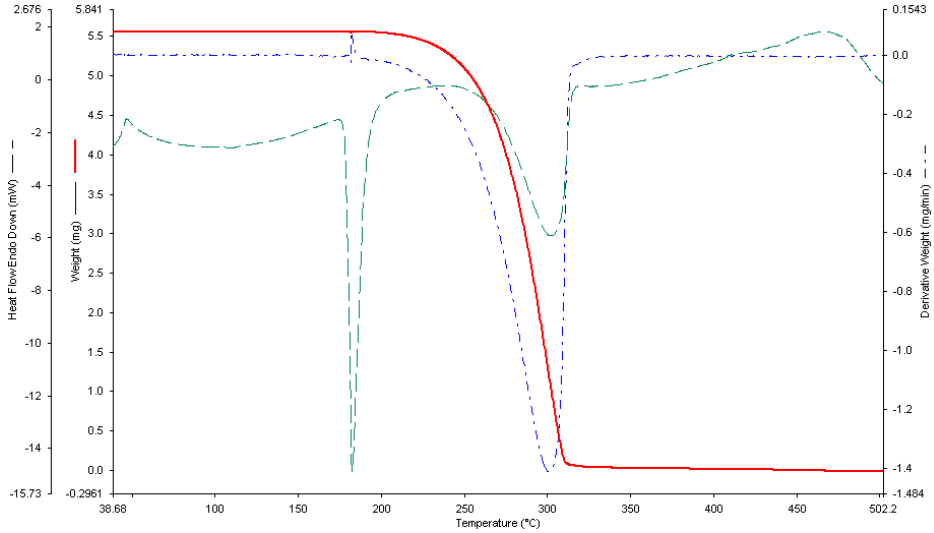

Fig. 1. TG/DTG/HF data of phenprocumonului

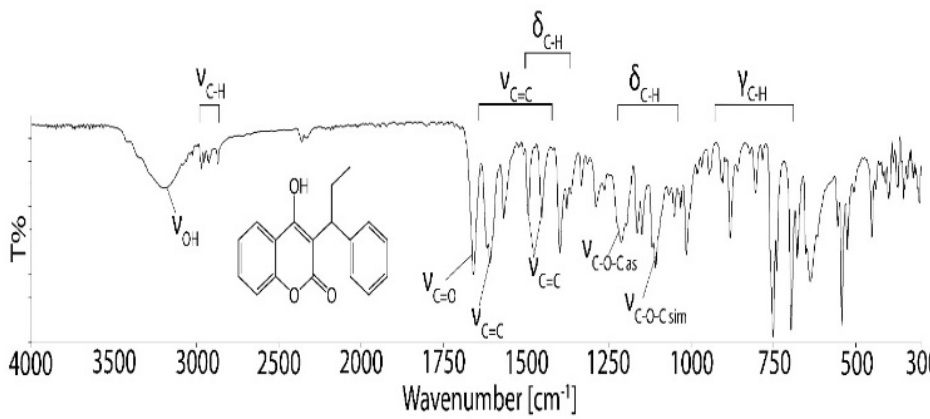

Fig. 2. FT-IR spectra of phenprocumonului

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Optimizing thermal condition in a patrol vessel engine room through ventilation strategy: onsite data analysis and numerical simulations

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Keywords: thermal comfort, heat stress, engine room, CFD simulation, onsite measurement

Effective heat stress management is essential to safeguard worker safety and well-being, particularly in high-temperature environments such as engine rooms. Proper control of heat stress not only reduces the risk of heat-related illnesses but also maintains productivity and prevents accidents. This study examines the thermal conditions within the engine room of a patrol vessel under two operational scenarios: (i) static condition with the engine running and (ii) moving condition. To address heat stress concerns, both onsite measurements and numerical simulations were conducted to analyse and optimize thermal conditions at various sampling points within the engine room. Onsite measurements included air temperature, radiant temperature, air velocity, relative humidity, clothing type, and work rate. Handheld digital anemometers, thermal imaging cameras, and wet bulb globe temperature (WBGT) meters were employed to assess airflow, radiant heat, and heat stress levels. The findings reveal that during the moving conditions, engine room temperatures exceeded 35°C, surpassing the ISO 8861:1998 recommended limits for optimal working conditions. This extreme thermal environment significantly increased heat stress risk, reducing the permissible working time to approximately 25.5 to 34.5 minutes, depending on the location within the engine room. 83% of sampling points were deemed unsuitable for performing work tasks due to high heat stress risk. To mitigate these risks, this study proposed a ventilation strategy based on numerical simulations. A full-scale (1:1) 3D model of the engine room was developed using computer-aided design (CAD) software, and computational fluid dynamics (CFD) simulations were conducted to analyse thermal and airflow distributions. The numerical results were validated against onsite measurements, ensuring the reliability of the simulation outcomes. The proposed ventilation strategy, which involved integrating additional air inlets on the wall

and ceiling (near the prime mover), demonstrated significant improvements. Air temperature reductions between 3.4°C and 3.8°C were observed, resulting in an increase in permissible working time to approximately 33 to 40 minutes. This intervention effectively reduced heat stress risk from a high to a medium level for ship crew members. This study provides valuable insights into optimizing engine room ventilation and highlights the importance of future research. Future studies should explore thermal comfort analysis, physiological responses to heat stress, and heat-related disorders. Additionally, integrating real-time air quality monitoring using IoT-based approaches and exploring heat stress control through digital twin applications could further enhance heat management strategies in engine room environments.

Acknowledgments

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T15: Materials science

Synthesis and characterization of FeNiMnAlCu high-entropy alloy for magnetic applications

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Keywords: solution combustion synthesis, high-entropy alloy, magnetic properties

The High-entropy Alloy (HEA) is a relatively new class of materials consisting of five or more major elements in equal or nearly equal atomic proportions. They become emerging advanced materials due to extraordinary mechanical properties, corrosion resistance, thermal stability, and other promising functional properties. Moreover, in the past few years, several research articles appeared that describe the excellent magnetic properties of HEAs. More than four principal elements help to tune the magnetic properties along with other properties, such a mechanical, corrosion, etc., which are required for industrial applications of magnetic materials. Among the various HEAs, FeNiMnAlCu HEA is prone to exhibit interesting magnetic behaviour due to the combination of magnetic (Fe, Ni) and non-magnetic (Al, Mn, Cu) elements. The magnetic properties of HEAs are highly dependent on the phase composition, microstructure, synthesis route, processing parameter, which can be tuned through the synthesis strategy. The solution combustion synthesis is a perspective and efficient method for preparing FeNiMnAlCu HEA and improving its magnetic performance.

The synthesis was carried out in aqueous solutions of the $Fe(NO_3)_3$-$Ni(NO_3)_2$-$Mn(NO_3)_3$-$Al(NO_3)_3$-$Cu(NO_3)_2$ - $C_6H_{12}N_4$ system, where the nitrates are oxidizers and $C_6H_{12}N_4$ (hexamethylenetetramine) is the organic fuel. The oxidizer-fuel ratio (ϕ) was controlled by these reactions:

$$Me(NO_3)_2 + \frac{1}{3}\varphi\, C_6H_{12}N_4 + 3(\varphi - 1)\, O_2 = Me + 2\varphi\, CO_2 + 2\varphi\, H_2O + \frac{4\varphi + 6}{3}\, N_2$$

$$Me(NO_3)_3 + \frac{1}{2}\varphi\, C_6H_{12}N_4 + 3(\varphi - 1)\, O_2 = Me + 3\varphi\, CO_2 + 3\varphi\, H_2O + (\varphi + 3)\, N_2$$

The effect of fuel quantity on the composition and microstructure of the combustion product was investigated. The optimal conditions according to initial mixture composition, pH of the solution and ambient atmosphere were found for the preparation of single-phase magnetic FeNiMnAlCu alloy.

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Statistical approach and computational tools for time temperature superposition principle

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Keywords: time-temperature superposition, master curve, functional data analysis, r software, computational statistics

This work approaches a new description of the Time Temperature Superposition (TTS) principle from a statistical perspective. Specifically, the present study contributes to the TTS issue in two ways. On the one hand, it describes, in the framework of Functional Data Analysis (FDA), the TTS principle and the master curve as the functional mean,

$$\psi(x,T)=\mathrm{E}(Y(x,T)),$$

of some viscoelastic property, Y, depending on time/frequency, x, at the required temperature, T. On the other hand, this work formally defines, explains, and applies the statistical model based on the very intuitive and descriptive MNAT method [1]. This approach consists in obtaining the shift factors and the master curve in a TTS analysis from the horizontal shifting of the first derivative function of viscoelastic properties. The statistical model based on the MNAT method provides shift factor estimations and smooth master curve estimates using B-spline fitting, with bootstrap confidence intervals. This technique has been used in diverse applications dealing with material reliability, such as life time estimations of adhesives in naval industry [2]. This procedure is implemented using the R open-source software [3] in the TTS package [4], which enable practitioners of academy and companies to apply the TTS principle in a free and totally reproducible way. The application of MNAT method through the TTS package is illustrated with different practical examples.

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Mass spectrometry evolved gas analysis as potential method to determined kinetics parameters for chrysotile dehydroxylation in cement-asbestos samples

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Keywords: chrysotile, cement-asbestos materials, thermal decomposition, dehydroxylation, kinetics

Asbestos containing materials were used in the past in many applications [1-2]. But in the first part of the 20th century, the danger resulting from using asbestos materials started to be known, especially their carcinogenic properties. This is the reason why asbestos materials have been recognized as hazardous waste and theirs use has been forbidden. Thermal treatment can be a promising option for end-of-life asbestos-containing materials deactivation including cement-asbestos products [3-5]. This is the main reason for undertaking this research in which kinetic data of the dehydroxylation of chrysotile $Mg_3(OH)_4Si_2O_5$ contained in cement-asbestos materials in the form of roof panels coming from different locations of Poland were tested and compared with kinetic data obtained for pure chrysotile. Because the effects resulting from the decomposition of the cementitious matrix dominated all obtained thermogravimetric curves the mass spectrometry evolved gas analysis data for released water were used for kinetic analysis. The Friedman (FM) method [6] was applied to determine the activation energy without the assumption of a reaction model. The dependences of the activation energy of chrysotile dehydroxylation on the degree of reaction obtained using the Friedman method are comparable for cement-asbestos materials and pure chrysotile. The use of mass spectrometry data for released water allows for the kinetic analysis of chrysotile dehydroxylation in the presence of other components undergoing thermal changes at the same temperature as chrysotile. The limitation of the method may be the small amount of chrysotile contained in the sample and, consequently, the small amount of water released during its dehydroxylation. The amount of water reaching the mass spectrometer must be much greater than the detection limit of the spectrometer so that the obtained signals can be used to estimate kinetic parameters. In our measurements, 5% of chrysotile in the cement-asbestos sample, the amount determined by X-ray diffraction (XRD), gave a released water signal suitable for further kinetic calculations. The applied method for determining the kinetic parameters of the chrysotile dehydroxylation reaction allows for studying the influence of the components contained in the cement matrix on the chrysotile dehydroxylation.

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Influence of environmental factors on the compatibility between prasugrel: excipients

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Keywords: prasugel, excipients, compatibility, biopolymers

This study investigates the impact of various environmental factors on the compatibility between prasugrel and various excipients. Prasugrel, a thienopyridine derivative, is widely used as an antiplatelet agent in the management of acute coronary syndrome. The compatibility between prasugrel and excipients is crucial for ensuring the stability and efficacy of the drug. Environmental factors such as temperature, humidity, and light exposure can significantly influence the interaction between prasugrel and excipients, potentially affecting the drug's stability, dissolution rate, and bioavailability.

The study employs a range of analytical techniques, including Fourier Transform Infrared Spectroscopy (FTIR), Differential Scanning Calorimetry (DSC), and High-Performance Liquid Chromatography (HPLC), to assess the compatibility of prasugrel with various excipients under different environmental conditions. The findings reveal that certain environmental factors can lead to the degradation of prasugrel, resulting in reduced efficacy and potential safety concerns. The study highlights the importance of optimizing storage conditions and selecting appropriate excipients to enhance the stability and performance of prasugrel formulations.

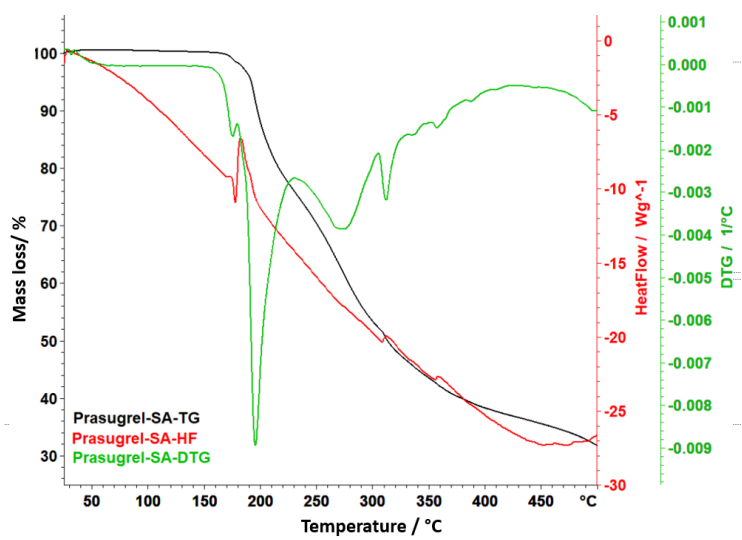

Fig 1. TG/DTG/HF curves for Prasugrel.

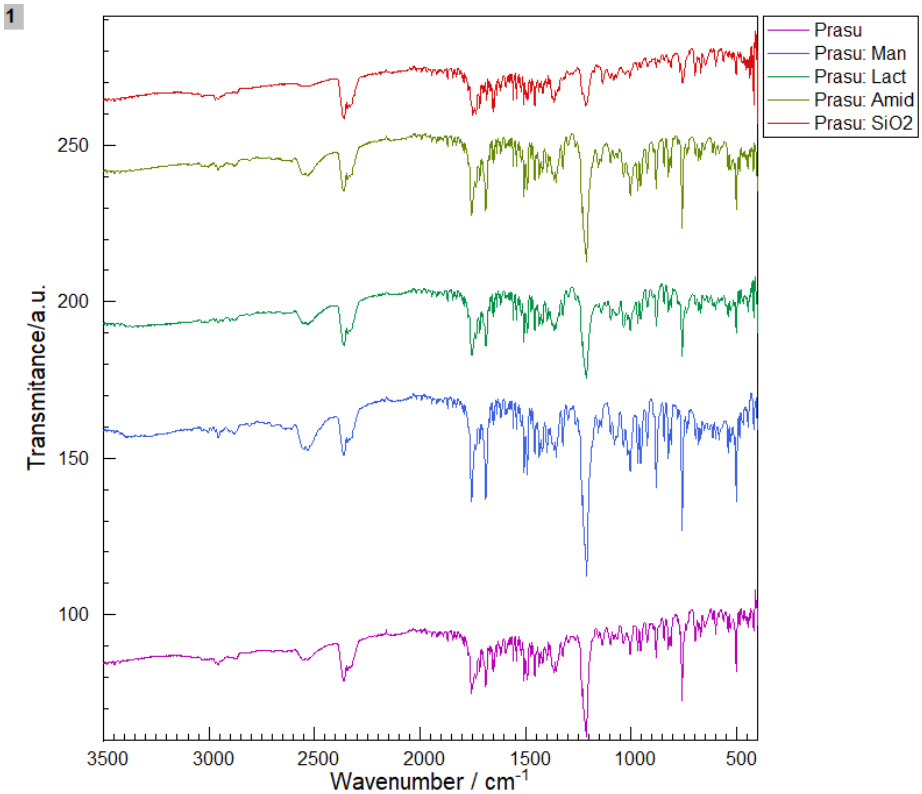

Fig 2. FTIR spectra for Prasugrel and excipients

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Adsorptive removal of Rhodamine 6G using KOH-activated hydrochar from spent coffee grounds: kinetics, isotherms, and thermodynamic analysis

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Keywords: hydrochar, spent coffee grounds, Rhodamine 6G, adsorption, kinetics, isotherms, thermodynamics, wastewater treatment

The exponential growth of the textile industry has significantly intensified dye pollution, with cationic dyes like Rhodamine 6G (Rh 6G) posing serious environmental and health risks. In this study, hydrochar derived from spent coffee grounds (SCG) an abundant and low-cost biomass was investigated as a sustainable adsorbent for Rh 6G removal from aqueous solutions. Hydrothermal carbonization was performed at 160–200 °C for 3–7 hours, followed by KOH activation to enhance surface functionality.

Comprehensive characterization using SEM-EDX, FTIR, XRD, TG-DTA/DTG-MS, and BET analysis revealed notable trends: SEM micrographs revealed a shift from macroporous to microporous structures with increasing temperature and residence time. EDX analysis showed a steady rise in surface carbon content indicating enhanced carbonization. FTIR spectra exhibited stronger O-H, C=C, and C=O bands at higher temperatures and residence time, reflecting increased surface polarity and oxygenated functional groups beneficial for dye adsorption. The disappearance of methyl-associated peaks confirmed degradation of caffeine-related compounds. XRD analysis showed a reduction in amorphous cellulose and enhanced ordering of graphitic structures. Thermal degradation profiles from TG-DTA/DTG-MS confirmed multi-stage decomposition of hemicellulose, cellulose, and lignin. BET measurements showed increase in surface area with increased temperature.

The adsorption kinetics were best described by the pseudo-second order and Elovich models, indicating chemisorption on heterogeneous surfaces. Isotherm studies revealed a shift from Freundlich to Langmuir behaviour with increasing temperature, while thermodynamic parameters ($\Delta G°$, $\Delta H°$, $\Delta S°$) confirmed spontaneous and primarily exothermic adsorption, except for one sample showing endothermic behavior. The adsorption was highly pH-dependent, with alkaline conditions favouring maximum dye uptake. These findings demonstrate the potential of SCG-derived hydrochar as an eco-friendly alternative for dye-contaminated wastewater treatment.

Thermal analysis of amphibole varieties of asbestos

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Keywords: amphibole asbestos, thermal decomposition, dehydroxylation

Thanks to their undeniably good strength properties, cement-asbestos materials (ACM) have been widely used as construction and insulation materials [1]. Their heyday ended with the discovery of their carcinogenic properties, which led to serious diseases in people exposed to asbestos during ACM production [2]. For many years, programs to safely remove asbestos from public spaces have been carried out in over 70 countries [3]. However, based on the assumptions of the circular economy, scientists are striving for effective disposal and recycling of asbestos fibres. Among the methods used, thermal degradation of asbestos fibres and their transformation into safe mineral forms is particularly beneficial [4]. The main raw material in cement-asbestos materials is chrysotile (asbestos from the serpentine group), whose thermal decomposition is already quite well known [5], but ACMs may also contain asbestos from the amphibole group, in particular crocidolite and amosite [6]. They are characterised by a different chemical composition, a various dehydroxylation temperature and a different course of thermal changes [7]. The characteristics and comparison of asbestos from the group of amphiboles such as amosite, tremolite, crocidolite, anthophyllite and actinolite are discussed in this research. The sense of the research stems from the need to characterise materials with carcinogenic properties, which, like chrysotile, are present in ACM, and are equally harmful to the environment and humans, but show completely different thermal properties during annealing. Since one of the ways to degrade the hazardous properties of asbestos is through its thermal treatment, thermal analysis studies (DTA/TG, DTG) up to 1400°C were used to characterise the fibres in terms of their behaviour during heating. Data obtained by the thermogravimetric method allowed us to determine thermal changes, in particular, related to dehydration, decarboxylation and dehydroxylation of materials. As a result of heat treatment, the samples underwent these processes in different temperature ranges, where special attention should be paid to the dehydroxylation temperature of amosite, tremolite and anthophyllite, which takes place at a temperature of about 1000°C, which is higher than for chrysotile (500-800°C). This should be considered when modelling the degradation process of asbestos fibres in ACMs containing them. Due to the high heating temperature, the melting points of the materials studied were also noticed.

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Modified layered double hydroxides as effective adsorbents of arsenate(V) and chromate(VI) anions

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Keywords: chromium(VI), arsenic(V), sorption, layered double hydroxide, LDH

Chromium and arsenic compounds are significant environmental pollutants. Their presence in the environment is mainly due to intensive human activity in many different fields of industry. They are highly toxic and have proven carcinogenic properties [1, 2]. Therefore, it is necessary to search for newer and more effective methods of their removal from polluted water and sewage. Materials from the group of layered double hydroxides, called "anionic clays", are well suited for use in this topic. Thanks to the great possibilities of modifying the structure of their layers and the interlayer space, they become a good adsorption material for undesirable anions.

In this study, the sorption of chromate(VI) and arsenate(V) ions on different Mg^{2+}/Al^{3+}-based layered double hydroxides was investigated. The basic carbonate-containing LDHs in which the Mg2+/Al3+ ratio was 2:1 or 3:1 were modified by introducing additional cations: Zn^{2+}, Cu^{2+} and Fe^{3+}. All materials were obtained by the co-precipitation method. Another modification was to replace CO_3^{2-} with Cl^- anions in the interlayer space of the synthesized LDHs. Then, sorption processes of arsenate(V) and chromate(VI) anions from aqueous solutions were performed on all prepared adsorbents. The influence of contact time, initial concentration and pH of solutions on the sorption efficiency of $HAsO_4^{2-}$ and CrO_4^{2-} ions on these materials was established.

The synthesized adsorbents were characterized by thermal analyses applying the thermogravimetric (TG) and differential scanning calorimetry (DSC) methods using the SETSYS16/18 analyzer (Setaram). The analyses were carried out before and after the As(V) and Cr(VI) ion sorption processes. Fourier transform infrared spectroscopy (FTIR) of obtained materials was performed using an Alpha spectrometer (Bruker, Inc., Germany) in the wavenumber range from 4000 to 450 cm^{-1}, with a resolution of 4 cm^{-1}. Powder X-ray diffraction (XRD) patterns were registered using a Rigaku MiniFlex II diffractometer. The concentration of Cr(VI) and As(V) ions in solutions was determined by the colorimetric methods based on 1,5-diphenylcarbazide dye and ammonium molybdate, respectively. The room temperature absorption measurements were performed on a JASCO V-660 UV-Vis spectrophotometer.

The adsorption processes of chromate(VI) and arsenate(V) anions were successfully carried out on all synthesized materials. Generally, higher sorption parameters were obtained for double layered hydroxides in chloride form, compared to carbonate one. Based on the analysis of the XRD data, it was found that in the case of carbonate-containing LDH, only surface adsorption of Cr(VI) and As(V) ions takes place. In the chloride form of the materials, ion exchange in the interlayer space also takes place. The best adsorption capacity towards the analyzed anions was demonstrated by LDHs containing Cu^{2+} and Zn^{2+} ions in their structure.

Thermal analysis confirmed the decomposition of all layered double hydroxides in a similar way, including its main stages [3]. Differences in the TG-DSC curves related to LDH modifications and the presence of adsorbed As(V) and Cr(VI) anions were observed.

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Thermal dependence of the structure in XFe_2O_4 (X=Co,Cu,Fe,Mg,Mn,Ni) high-entropy spinel ferrites synthesized via reactive flash sintering

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Keywords: reactive flash sintering, spinel-type ferrite, high entropy oxides, thermal stability

Since the introduction of high entropy alloys in 2004 [1], interest in multicompontent materials has surged within the materials science community. This field has expanded to include high-entropy oxides (HEOs), demonstrating that the high-entropy concept can be successfully applied to ceramics as well [2]. Achieving a single-phase structure in HEOs requires careful selection of synthesis methods, as these influence powder morphology, elemental distribution, particle size, and overall processability.

Among various techniques, Reactive Flash Sintering (RFS) has emerged as a promising method for synthesizing HEOs. As a non-equilibrium process, RFS enables the formation of metastable phases that conventional techniques cannot achieve. Given its out-of-equilibrium nature, understanding the thermal stability of materials synthesized by RFS is crucial. This work reports the concomitant synthesis and sintering of two HEOs, $(Mn_{0.2}Co_{0.2}Ni_{0.2}Cu_{0.2}Fe_{0.2})Fe_2O_4$ and $(Mn_{0.2}Co_{0.2}Ni_{0.2}Cu_{0.2}Mg_{0.2})Fe_2O_4$, into single-phase spinel compounds using RFS [3]. X-ray diffraction (XRD) confirmed the macroscopic single-phase spinel structure, while electron microscopy combined with energy-dispersive spectroscopy (EDS) mapping verified the random distribution of constituent elements. A combination of in-situ and ex-situ XRD analysis, along with calorimetric experiments, revealed a two-step destabilization process of the spinel structure upon heating. In the first step, above 650 ºC, a Fe_2O_3 begins to coexist with the spinel phase. Above 900ºC, a Cu-based oxide precipitates, while the Fe_2O_3 phase disappears. Results obtained from the different techniques are consistent, with EDS mappings confirming the precipitation of distinct phases during the thermal treatment.

HEOs with spinel structures synthesized via conventional methods, such as solid-state reactions, require high temperatures and extended reaction times, potentially leading to instability. In contrast, non-equilibrium techniques like RFS offer a valuable alternative for producing these materials while maintaining structural integrity.

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Analysis of the thermal properties of magnesium alloy with the addition of noble and rare earth elements

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Keywords: Mg-based alloys, mechanical alloying, DSC

The study of the thermal properties of magnesium alloys is essential for several reasons, especially in their applications in the aerospace, automotive, biomedical, and electronics industries. Thermal studies allow us to determine the temperature range in which the alloy retains its mechanical and structural properties. Differential scanning calorimetry (DSC) will enable us to study phase transitions, e.g., melting, crystallization, or precipitation of reinforcing phases.

This work aims to produce and characterize biodegradable metal materials based on magnesium with noble metal (silver) and rare earth (erbium) additives using powder metallurgy. The purpose of adding additives in the form of precious metals and rare earth elements to the alloy is to create a specific structure ensuring optimal mechanical and anti-corrosion properties. The alloy synthesized by mechanical alloying was subjected to tests such as analysis of the structure and phase composition (X-ray diffractometry and scanning electron microscopy). The particle size distribution in the alloys was determined using the laser particle size measurement method. The thermal characteristics of the powders were investigated using differential scanning calorimetry (DSC).

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Thermal analysis of an iron-based alloy produced by powder metallurgy

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Keywords: Fe-based alloys, MA, DTA

Iron-based alloys are mainly used in advanced functional materials, especially where magnetic, tribological, structural, or wear-resistance properties are important. The paper presents the results of studies of alloys with the compositions $Fe_{82}B_{16}La_2$ and $Fe_{82}B_{14}La_4$ produced in high-energy milling. The powders were milled for 10, 30, and 50 h, with each hour's break being followed by a 0.5 h break. The morphology of the obtained alloys and the chemical composition were examined using a high-resolution scanning electron microscope (SEM). Maps of the distribution of elements in powder particles were also made. The X-ray diffraction method (XRD) examined structural studies of powders after milling. The $Fe_{82}B_{16}La_2$ and $Fe_{82}B_{14}La_4$ alloys were also subjected to differential thermal analysis (DTA) tests, which determined the temperatures at which the Fe_2B iron boride phases are formed, which are responsible for increased hardness and abrasion resistance, and the temperature range of phase transformations occurring in the Fe-B-La alloys.

The presence of boron and iron borides in alloys significantly increases hardness and abrasion resistance. Lanthanum can improve the grain boundary structure and stabilize phases, affecting durability and their resistance to degradation. They are used to produce cutting tools, engine components, pistons, and wear-resistant coatings of working surfaces (e.g., in metallurgy and heavy industry).

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The influence of temperature on thermal and mechanical properties of beech-pu-beech joints

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Keywords: polyurethanes, FPUR, RPUR, DMA, thermal analysis, thermal conductivity, thermal diffusivity, thermal stability, thermal resistance

An important element of wooden structures is adhesive joints based on polyurethanes, containing various amounts of flame retardant additives, modifiers of mechanical properties and increasing resistance to ageing. In this work, PS, PTS, and PTS polyurethanes were modified, and the ratio of soft to hard segments differed. It allows you to control these adhesive agents' mechanical properties and thermal stability and dissipate vibration energy in the structure. The dissipation of the supplied external energy in the polymer structure is an important element of glued wood joints due to the vibrations of the entire structure. This parameter depends on the structure of the adhesive, which is directly related to the mechanical properties, and on the thermal properties, which affect the rate of structural changes of the connection. For this reason, beech-polyurethane-beech glued joints were prepared and first subjected to dynamic mechanical analysis.

The influence of the composition of adhesive agents on the transformation temperature, the value of the storage modulus, loss modulus and phase angle was determined. The tests were carried out in the direction perpendicular and parallel to the bonded connection. The influence of polyurethane thickness on the DMA analysis result was also determined. DMA measurements were carried out at various frequencies at a temperature ranging from -100°C to 150°C. The measurement results were correlated with sample layers dimensions. The performed thermomechanical analyses were correlated with heat transport through the three-layer system at temperatures from room to 150°C. All of the 3L measurements were compared and explained by the analysis of single constituent layers, so PUs and beech wood.

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Thermophysical and thermomechanical properties of epoxy resin – boron carbide – hexagonal boron nitride composites

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Keywords: epoxy resin, composites, boron carbide, B4C, hexagonal boron nitride, h-BN, DMA, LFA, thermal expansion

In recent years, publications on adding boron carbide to resins have begun to appear. Boron carbide is a low-density, rigid material that can increase mechanical properties competitively. Therefore, it can affect the hardness or abrasion of the material. In addition, it undergoes passive oxidation at elevated temperatures to be used as a fire retardant. Papers indicate that this filler can be used as a radiation shielding component. Typical B_4C additive was up to 5% by weight. In one paper, which was found, in the case of radiation shielding, a concentration of 20 wt.% of boron carbide was examined. On the other hand, the addition of hexagonal boron nitride can positively influence thermal conductivity and electrical resistivity, decrease friction coefficient and improve the thermal stability of the polymer. The h-BN was added in quantity up to 18.5 vol.%. The paper talks about the self-healing of epoxy materials containing this boron nitride. That is why we focused on composites containing high concentrations of boron carbide and boron nitride. For this purpose, the high-viscosity resin was mixed with boron-based ceramic phases, giving the following volume concentration: 2.5, 5, 10 and 20% of boron carbide, 2.5, 5, 10 and 20% of hexagonal boron nitride and a mixture of ceramic phases in quantity B4C/hBN equal to 1.25/1.25, 2.5/2.5, 5/5 and 10/10. Such compositions allowed us to investigate the influence of fillers on dispersion rheology and the thermophysical and thermomechanical properties of composites. The thermal behaviour of epoxy matrix composites was studied using thermal stability in protective and air atmosphere by differential scanning calorimetry, thermal expansion by dilatometric measurements, thermal diffusivity and conductivity by laser flash analysis method and dynamic mechanical analysis of storage and loss modulus by DMA apparatus. Due to B4C and h-BN fillers, these new materials can interest researchers as a part of a passive shield for army purposes.

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Microstructural and thermal investigations of natural fluorapatite via long time tribochemical activation

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Key word: tribochemical activation, isomorphic substitution, carbonate apatite, quartz, thermal analysis

The present work investigates the effect of dry mechanochemical activation, known as tribochemical activation, on natural fluorapatite originating from Tunisia, North Africa. Tunisian phosphorite is characterized by a total phosphate content recalculated as $P_2O_5^{tot}$ - 27.6%, Ca as CaO - 50.0%, low quartz content - 3.6%, calcite - 2.9%, dolomite - 1.2%, etc. This raw material has traditionally been used for the production of phosphate fertilizers by the classical acid method. Tribochemical activation is a method of treating conventional and low-grade raw materials as a method of enhancing the reactivity of chemically resistant natural apatite [1, 2]. This method is an environmentally friendly alternative as it eliminates the disadvantages of conventional methods, namely the release of gaseous and solid technogenic products [3]. The activation was performed via planetary mill with plain steel grinding bodies of varying diameters (3-20 mm) for a relatively long activation time of 150 minutes.

The aim of the present work is to examine the microstructural transformations in the parameters of the crystalline state of the main mineral apatite while varying the size of the grinding bodies and keeping constant the other activation parameters - loading of the tribo-activator at maximum speed, type of grinding bodies, and activation duration. Additionally, the activation effect on the structural-phase transformations occurring in the impurity minerals - free calcite/dolomite, quartz is examined. Their influence on the thermal behavior of the apatite is also assessed.

The tribochemical activation effect is observed by using a complex of analytical methods, such as chemical analysis, X-ray fluorescence (WD-XRF) analysis, X-ray powder diffraction (XRD), Fourier transformed infrared (FTIR) measurements, and thermal analysis (TG/DTG-DSC) coupled with Pfeiffer Omnistar Mass Spectrometer.

The results show that the activation has the following impact at micro-level: (i) microstructural transformations and induced defects; (ii) isomorphous transformations; and (iii) solid-phase synthesis reactions. They present a correlation in the behavior of the studied samples in regard to their quartz content and bonded or non-bonded carbonate ions. After tribochemical activation of the raw samples, A-and A-B type carbonate-apatite are formed. The new isomorphic phases (A-and A-B type carbonate-apatite) are decarbonized at temperatures of about 780-850 K and 1050-1100 K. In the presence of quartz, the decomposition temperature for carbonate ions in the A-site increased. In addition, the moisture and higher quartz content in the samples leads to a shift in the dehydroxylation temperature.

The obtained results have practical significance for the development of eco-agriculture - production of fertilizers, soil improvers, and activators.

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Study of precursors for the preparation of doped catio$_3$ pigments via sol-gel process

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Keywords: inorganic pigments, sol-gel method, thermal analysis, doped $CaTiO_3$

Calcium titanate ($CaTiO_3$) is an attractive candidate for developing cool pigments due to its stable crystal structure and to modify its optical properties. However, its wide band gap of approximately 3.5 eV (UV light region), arises from the significant energy gap between the O 2p valence band and the Ti 3d conduction band, restricts its use in optical, pigmentary, and luminescent applications. To overcome this limitation, doping the structure has proven to be an effective strategy. This approach enables the material to absorb a broader spectrum of wavelengths, including the visible range (400–700 nm), thereby enhancing its physical and chemical characteristics for pigmentary purposes [1-2].

Doped $CaTiO_3$ pigments with the transition metals ($CaTi_{0.9}M_{0.1}O_3$, M = Mn, Co, Ni, Fe) were synthesised via a citrate sol-gel method using nitrate precursors, followed by a high-temperature calcination process. The synthesis involved dissolving calcium nitrate in 60 ml of absolute ethanol with constant stirring of 190 rpm and heating at 60±3 °C. Citric acid monohydrate was then added as chelating reagent. Separately, the nitrate salts of the transition metals (Mn^{2+}, Co^{2+}, Ni^{2+}, Fe^{3+}) were dissolved in 20 ml of absolute ethanol, and then added to the calcium-chelate solution. Finally, titanium isopropoxide was added dropwise under constant stirring, with the solution maintained at 60±3 °C for 2 hours, forming a viscous gel. The gel was dried at 80 °C for 48 hours and manually milled before undergoing a two-step calcination process: an initial step at 350 °C to remove organics, yielding a brownish precursor, followed by final calcination at 900–1200 °C for 8 hours to form crystalline phases. To optimize the particle size, the calcined powders were wet-milled in a planetary mill with zirconia balls in an ethanol medium, using controlled milling parameters: 10-minute duration, a spinning speed of 200 rpm, and a ball-to-powder weight ratio of 8:1 [1].

The thermal behaviour and reactivity of the dried precursors were analysed using simultaneous DSC/TG. Based on mass loss and thermal events, the processes occurring in the intermediates were studied and the optimal synthesis temperatures were determined. The DSC curves exhibited exothermic peaks within the range of 200−600 °C. These peaks are corresponded to the combustion of organic and nitrogen-containing intermediates from sol-gel synthesis [3]. These exothermic peaks were accompanied by significant mass loss, ranging from -72% to -78.5%. In the temperature range of 630−660 °C, the crystallization and the formation of doped $CaTiO_3$ structure were observed, as confirmed by XRD results of samples calcined for 1 minute at 650 °C and 700 °C. The obtained pigments were subjected to comprehensive evaluations, including thermal stability up to 1500 °C, optical and colour properties, and phase composition analyses.

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Effect of water leaching on composition and thermal properties of wood barks

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Keywords: wood bark, water leaching, TG/MS

Renewable energy sources, including biomass via modern bioenergy, help reduce greenhouse gas emissions by partially replacing fossil fuels. Biocarbon produced by biomass pyrolysis has diverse applications requiring specific chemical and physical properties. Its composition and the amount of volatile matter are very important properties for the biocarbon utilisation, while high fixed carbon yield is desirable for an economical production. Low ash and inorganic content are critical especially in the case of producing biocarbon for metallurgical use. Stem wood produces high-quality biocarbon but its availability is limited and it is costly. Wood bark, a wood industry by-product, is a cheaper alternative compared to stem wood but has much higher ash content where some elements, e.g. alkali metals, need to be reduced for producing biocarbon to be used in metallurgical applications.

In this work, the effect of water leaching on the composition and thermal properties of wood bark was tested for the bark of birch, spruce and pine, which are common wood species in the northern hemisphere. Dried wood bark samples were ground to 1 mm particle size and were leached with deionized water at room temperature (25 °C) without stirring and at 60 °C with continuous stirring. The solid yield of the dry leached bark and the amount of dried leachate were measured.

As a result of leaching, moderate decrease in the ash content of the bark samples was observed, while the solid yield of the leached bark was around 90%. The effect of leaching temperature and the stirring on the change in ash content did not show a clear trend. The difference between the mass loss and the ash content decrease indicates that significant amount of organic matter was also extracted. Inductively coupled plasma optical emission spectroscopy (ICP-OES) was used to follow the efficiency of water leaching on the inorganic content removal. The proportions of cellulose, hemicellulose and Klason lignin in both untreated and water-extracted samples were determined after acidic hydrolysis and HPLC analysis. The influence of water extraction on the characteristics of wood barks was studied by thermogravimetry combined with mass spectrometry (TG/MS). The changes in the shape of DTG curves reflects the modified composition and thermal properties of the leached bark samples. The TG/MS ion intensity curves of raw bark, leached bark and extract samples reveal information about the chemical composition and decomposition temperature of the extracted organic material.

Innovative temperature-dependent studies on the structural and thermal properties of rigid and flexible polyurethane adhesives

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Keywords: polyurethane adhesives, thermal analysis, FTIR, Raman spectroscopy, XRD, TG-FTIR, temperature-dependent studies

Polyurethane (PU) adhesives are widely used in industrial applications due to their adaptability, mechanical strength, and thermal properties. This study explores the behavior of rigid polyurethane (RPU) and flexible polyurethane (FPU) adhesives by analyzing four structurally distinct types: PT, PST, PTS, and PM. The primary objective was to evaluate their structural and thermal performance over a wide temperature range.

The adhesives were characterized using Fourier-transform infrared spectroscopy (FTIR), Raman spectroscopy, X-ray diffraction (XRD), and thermogravimetric analysis coupled with FTIR spectroscopy (TG-FTIR). FTIR and Raman spectroscopy helped to understand the molecular structure and interactions between molecules, showing differences in hydrogen bonding and how the phases separate in rigid and flexible polyurethanes. XRD analysis measured how ordered the material is, showing that crosslinking and phase distribution changes affect the adhesive properties. Thermal stability and decomposition mechanisms were investigated using TG-FTIR, identifying differences in degradation pathways and emission profiles.

The findings indicate that rigid PUs (RPU) exhibit greater thermal stability and lower molecular mobility than flexible PUs (FPU), mainly due to their higher crosslinking density. Specific functional groups in PST and PTS formulations enhance phase separation, increasing structural rigidity and thermal resistance. Conversely, with its more flexible molecular architecture, PM-type polyurethane shows superior elasticity but a lower decomposition onset temperature. Quantitative analysis revealed that RPU materials exhibited degradation onset temperatures above 300°C, with weight loss occurring in multiple stages, indicating a stepwise decomposition mechanism. In contrast, FPU samples degraded at lower temperatures (~250°C) and followed a more continuous thermal degradation profile. XRD results confirmed that the increased crystallinity in RPU materials resulted in higher mechanical

stiffness, correlating with Raman spectral data showing more pronounced hydrogen bonding in these structures. The integration of TG-FTIR further allowed the identification of volatile decomposition products, with rigid PU adhesives releasing primarily carbonyl and isocyanate compounds, whereas flexible variants exhibited increased hydrocarbon emissions.

These studies were perform to better understand the thermal performance of PU adhesives and their practical application in wooden constructions, where strong and durable bonding is required under varying environmental conditions. The study highlights the role of temperature-dependent structural changes in optimizing PU adhesive performance in wood-based structures.

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Additive manufacturing of glassy-clay fertilizer carriers for controlled nutrient release

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Keywords: 3D printing, clay-based materials, fertilizer carriers, mixed-layer clay minerals, sustainable agriculture

Contemporary agriculture demands innovative solutions that enhance fertilizer efficiency while minimizing environmental impact. One such solution is the production of selective, glassy fertilizer carriers using 3D printing technology based on raw materials from mineral clay. Clays, rich in minerals such as kaolinite, illite, and smectite, are an excellent base for this purpose due to their physicochemical properties.

This study meticulously developed a slip-casting mass from raw clay materials with an innovative glassy fertilizer. It is a multi-stage process requiring precise preparation of both the raw materials and the slip itself. The research showed that each stage of the work performed plays a significant role in ensuring the quality of the final product. In its final form, this product can be used for innovative horticultural applications. The first step involved the selection of appropriate clay raw materials. Particular attention was paid to plasticity, fluidity, and density parameters, which are key factors dependent on the mineral composition, particle size distribution, and purity of the raw materials. Next, the raw materials underwent milling and sieving processes. Milling reduced the particle size of the raw materials, facilitating thorough homogenization of the raw material mixture and the removal of larger undesirable grains and aggregates in the subsequent preparation stage.

The next step was the preparation of an aqueous suspension, known as the slip. That is why the clay raw materials were mixed with a precisely determined amount of water and optimized experimentally to ensure the slip's optimal consistency. At this stage, the slip underwent another homogenization process. Subsequently, an innovative multi-component glassy fertilizer was introduced into the slip. This additive, a special type of glass with a precisely defined chemical composition, had been previously milled to the required particle size. The addition of finely milled powder to the slip was carefully controlled to ensure the uniform distribution of the fertilizer material within the slip.

The slip was utilized in an additive manufacturing (3D printing) process following preliminary laboratory tests. The designed 3D model, which represents the desired structure of the final product, facilitated the fabrication of a ceramic-glassy structure with precise control over the material's porosity and the formation of a rigid structure. This structure was then subjected to thermal treatment in a chamber furnace.

A range of advanced analytical techniques was employed to examine the properties of the engineered material, including X-ray diffraction (XRD), differential scanning calorimetry and thermogravimetry (DSC-TG), mechanical strength testing, and scanning electron

microscopy coupled with energy-dispersive spectroscopy (SEM). All thermal studies were performed in the Faculty Thermophysical Research Laboratory of the Faculty of Materials Science and Ceramics, AGH University of Krakow.

The results indicate that applying 3D printing technology combined with clays rich in minerals such as kaolinite, illite, and smectite enables the production of fertilizer carriers with high micro- and macroelements in their composition. The proposed innovative solution can potentially revolutionize sustainable agriculture. Integrating modern methods into studying these materials facilitates optimizing the production process and adapting new types of materials to perform multidimensionally in their action fertilizer materials.

Acknowledgments

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Thermal analysis (TG and CRTA) as a non-conventional analytical technique in microplastic detection

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Keywords: thermogravimetry, controlled-rate thermal analysis (CRTA), microplastic

The detection and identification of micro- (and nano)plastics in our environment (soil, water, air) is essential for mapping their effects on living organisms, assessing risks and developing mitigation and prevention procedures. To realistically assess adverse effects, we need to know not only their quantity, but also their size distribution and chemical composition [1]. Today, the state-of-the-art method for the chemical identification of microplastics is vibrational spectroscopy (μFTIR and μRaman spectrometry) [2]. At the same time, an appropriate sampling method and a standardised sample preparation procedure are prerequisites for reliable measurements, which is quite difficult for samples containing interfering components. The organic matter content of soil or compost samples makes it difficult to evaluate the IR/Raman spectra of the plastics, so they should be separated before analysis [3, 4]. However, separation methods are not perfect and can lead to losses, e.g. filtration losses or, chemical degradation caused by the digestion agent [5]. Non-conventional methods that require simpler sample preparation, such as thermal analysis, may then become more important. Although thermogravimetry does not always allow chemical identification, it can also be used as a preliminary analysis for vibrational spectroscopic detection.

In this work, we investigated the possibility of detecting (micro)plastics within a compost sample matrix using thermogravimetric methods. Although the technique provides only limited chemical identification (only if the thermal degradation of the plastic contaminant takes place in a discrete thermogravimetric range), it can be an advantageous solution due to the simple sample preparation (practically only particle size classification is required). Detectability of two types of degradable plastic bags (PE and PLA-based) in household compost were investigated. In the experiments, bag-compost samples of different proportions were prepared and the detection limit of the thermogravimetric technique were tested. For the closely overlapping decomposition steps, the specific CRTA (controlled-rate thermal analysis) measurement method was used. CRTA is advantageous in cases where the thermal decomposition of the plastic of interest (e.g. PLA) strongly overlaps with the thermal decomposition of the organic matter in the compost.

Acknowledgments
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Magnetic high-entropy alloys by aluminothermic reduction process

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Keywords: permanent magnets, high-entropy alloys, self-propagating high-temperature synthesis, exothermic reaction

Permanent magnets (PMs) convert electrical energy into mechanical motion and are widely used in renewable energy systems (e.g., wind turbines, wave energy converters) and sustainable transportation technologies (e.g., electric vehicles). The most efficient PMs are based on rare-earth elements (REE), defined by their high flux density (remanence, B_r) and energy density ($(BH)_{max}$). However, the criticality of REE, due to supply risks, price volatility, and environmental impacts, necessitates reducing their use in energy and transportation applications. The increasing demand for wind power generators and electric vehicles over the next decade intensifies this challenge. Innovations in magnetic materials are vital, particularly to develop rare-earth-free or rare-earth-lean magnets with energy products between 55 and 220 kJ/m³, addressing the need for sustainable alternatives in these strategic sectors [1].

High-entropy alloys (HEAs) are advanced materials composed of five or more principal elements in near-equiatomic proportions, resulting in high configurational entropy that stabilizes their microstructures [2]. Their unique properties stem from the complex interplay of elements, leading to lattice distortion, sluggish diffusion, and cocktail effects. Magnetic HEAs, a subclass designed for magnetic applications, combine multiple elements to tailor magnetic properties. Their complex compositions influence magnetic interactions, phase formation, and electron density, making them promising candidates for next-generation magnetic materials. Currently, vacuum arc melting and mechanical alloying are the primary methods for synthesizing HEAs. However, these techniques involve high costs due to expensive raw materials and significant electrical power consumption.

To address these limitations, self-propagating high-temperature synthesis (SHS) or combustion synthesis emerges as a cost-effective, rapid, and sustainable alternative [3]. Additionally, SHS offers greater flexibility in producing alloys with customizable phase and structural characteristics. In this work, to produce an equimolar FeCuNiMnAl HEA using the SHS method the mixture of both elements (Cu, Mn, Al) and oxides (Fe_2O_3, NiO) was selected. The exothermic Me_xO_y+Al reaction enabled the successful execution of the combustion wave propagation. As a result of the aluminothermic reduction a high-temperature, multi-component melt separation occur due to large difference in densities of the alumina slag and target alloy under normal gravitational conditions. The optimal conditions for achieving complete

phase separation were identified according to initial mixture composition and sample geometry. Magnetic properties and oxidation behavior under linear heating conditions of the final product were evaluated.

Acknowledgments
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T16: Metals, alloys, intermetallics

Thermal analysis and defect reduction in Al/Cu hybrid rotor casting using computational simulation and optimized heating channel design

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Keywords: Al/Cu hybrid rotor, high-pressure die-casting, cold shot defect, heat transfer coefficient, computational casting simulation

Recent advancements in induction motor design have emphasized improving energy efficiency, particularly through the implementation of hybrid aluminum-copper (Al/Cu) rotors. Copper's significantly higher electrical conductivity compared to aluminum enables reduced I^2R losses and enhanced motor performance. In Al/Cu hybrid rotors, copper bars are inserted into the laminated core slots and electrically bonded by aluminum end-rings formed via high-pressure die-casting (HPDC). This process efficiently combines the high conductivity of copper with the castability and cost-effectiveness of aluminum. HPDC is the most effective method for manufacturing such hybrid rotors. However, the rapid injection of molten aluminum can result in casting defects—most notably cold shots—caused by incomplete fusion of solidifying metal. These defects, often observed at the copper–aluminum interface, are associated with localized drops in melt temperature and can degrade both mechanical strength and electrical performance. Despite previous optimization efforts, cold shot defects persist even under controlled casting conditions due to thermal mismatches between materials and inadequate preheating. This study proposes an integrated methodology to analyze and reduce cold shot defects in Al/Cu hybrid rotor die-casting. The approach combines heating channel design, computational casting simulation, and the definition of interfacial heat transfer coefficients (HTCs). Six HTCs were applied to key interfaces including the mold, insert core, copper bars, and aluminum end-rings. MAGMASOFT® casting simulation software was used to perform thermal and filling analyses to evaluate melt flow and temperature distribution. Two heating system configurations—linear and circular—were simulated to assess their impact on thermal uniformity and defect formation. Results indicate that maintaining the appropriate preheat temperature of the copper bars and the laminated core is essential to prevent premature solidification and ensure complete fusion. Among the two, the circular heating system showed superior thermal distribution and reduced defect incidence. The findings highlight the importance of thermal control and HTC modeling in improving casting soundness. The proposed simulation-driven method serves as a reliable framework for identifying key process parameters, optimizing die design, and minimizing defect formation in the manufacturing of high-efficiency Al/Cu hybrid rotors.

Acknowledgments
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Precipitation-driven thermal diffusivity behavior of Al-6Si-0.4Mg-0.9Cu-(Ti) alloys for automotive engine applications

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Keywords: thermal diffusivity, Al-Si-Mg-Cu-(Ti) alloy, precipitation hardening, automotive engine components, heat treatment

In response to increasing demands for fuel efficiency and reduced greenhouse gas emissions, the automotive industry has progressively adopted lightweight materials such as aluminum alloys for structural and engine components. Among these, Al-Si-Mg-based alloys are particularly favored for critical engine parts such as cylinder heads due to their excellent thermal conductivity, castability, and high-temperature mechanical stability. Thermal diffusivity, a key property influencing heat dissipation efficiency, plays a critical role in maintaining thermal balance and mitigating thermal fatigue and hot spot formation in internal combustion engines [1-4]. However, the thermal diffusivity behavior of precipitation-hardened aluminum alloys in the practical service temperature range of 200–300 °C remains insufficiently characterized. This study aims to investigate the precipitation-dependent thermal diffusivity behavior of Al-6%Si-0.4%Mg-0.9%Cu-(Ti) alloys subjected to various heat treatment conditions, including solution treatment, quenching, and artificial aging. A series of alloys with and without Cu and Ti additions were cast, heat treated, and analyzed to examine their microstructural evolution, precipitation behavior, and thermal transport properties. The thermal diffusivity was measured using a laser flash analysis (LFA) system (Netzsch LFA457) from room temperature to 500 °C. Differential scanning calorimetry (DSC) and microstructural analysis (optical microscopy and EDX) were conducted to correlate the formation of metastable and stable precipitates with changes in thermal diffusivity. The results show that in all Si-containing alloys, thermal diffusivity did not decrease linearly with temperature, espechotially between 200 and 300 °C, where multiple exothermic peaks associated with the precipitation of β″-Mg_2Si, θ′-Al_2Cu, Q′, and Si phases were observed. The Cu-containing alloys exhibited distinct exothermic peaks at higher temperatures compared to Cu-free alloys, indicating delayed precipitation and improved thermal stability. Furthermore, the Ti-free 9C0T alloy demonstrated superior thermal diffusivity at all temperature ranges compared to the Ti-added 9C2T alloy, suggesting that Ti addition may slightly impede thermal transport due to its influence on precipitate distribution and morphology. Microstructural analysis confirmed that solution treatment promoted the spheroidization of eutectic Si, while aging led to the precipitation of nanoscale phases responsible for strengthening and altering thermal behavior. The aged samples at 220 °C showed higher thermal diffusivity than those aged at 180 °C, highlighting the impact of precipitation kinetics and phase evolution on thermal transport. In conclusion, this study elucidates the critical role of precipitation behavior in determining the thermal diffusivity of Al-6Si-0.4Mg-0.9Cu-(Ti) alloys within the operating temperature range of automotive engine components. These findings provide valuable insights for optimizing alloy design and heat treatment strategies aimed at enhancing thermal management and service reliability of lightweight aluminum components in the automotive industry.

Acknowledgments
This study has been conducted with the support of the Korea Institute of Industrial Technology as "Support program for technological advancement of plastic working & surface treatment in Jeonnam province.

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Properties of bulk metallic glasses $MG_{66}ZN_{30}CA_4$ for biomedical application

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Keywords: corrosion test, bulk metallic glasses, magnesium alloys, mechanical properties

In connection with the development of various fields of medicine, especially with the emergence of regenerative medicine, there has been a need to produce new materials that must be biocompatible, and increasingly also bioactive. Thanks to the development of biomaterials engineering, it has become possible to obtain bioactive material. This allows for the option to use a biomaterial that stimulates the regeneration of damaged tissue. Such materials are often made from calcium phosphates, e.g., hydroxyapatite or bio-glass, as these materials directly bond with bone. Biodegradable metals are another actively researched group of materials that, compared to polymers, have mechanical properties similar to bone. Magnesium and its alloys began to be considered at the beginning of the 21st century. Any material that is regarded as a biomaterial must meet specific requirements regarding its physical, mechanical, and chemical properties in order to be classified as biocompatible. For example, the material must be sufficiently durable to withstand physiological loads, be resistant to unwanted degradation or corrosion, and must not be carcinogenic, immunogenic, leukotactic, etc. Many factors, such as the size of the implant, shape, material composition, or roughness, affect the biocompatibility of the implant. Currently, magnesium-based alloys represent a new group of potential materials for short-term bioresorbable implants due to their biocompatible chemical composition. Research is being conducted on alloys including those with the composition Mg-Zn-Ca along with various alloying additives, such as rare earth elements. These are both amorphous and crystalline alloys; however, the amorphous materials after annealing at various temperatures of the $Mg_{66}Zn_{30}Ca_4$ alloy have not been studied. Nevertheless, there has been no actual application of either amorphous or crystalline alloys for resorbable biomedical implants to date.

Enhancement of high-pressure die-casting mold durability using laser cladding with stainless steel based coating material

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Keywords: die-casting, laser cladding, mold, deposition, thermal fatigue, aluminum alloy

The surface of high-pressure die-casting (HPDC) molds is subjected to repeated thermal cycling due to rapid heating by molten aluminum during injection and subsequent cooling by internal cooling systems and mold release agents. This cyclic thermal stress accumulates over time, leading to plastic deformation and surface degradation caused by thermal fatigue. SKD61 (STD61), the most commonly used steel for HPDC molds, exhibits limited resistance to thermal fatigue, soldering, and corrosion under high-temperature and high-pressure casting conditions. These degradation mechanisms reduce mold service life, increase production costs, and contribute to higher unit costs in aluminum casting operations. To improve mold durability, recent studies have focused on applying stainless steel (SUS)-based materials with superior corrosion and soldering resistance. Aluminum HPDC processes are particularly vulnerable to thermal fatigue due to the mismatch in thermal expansion coefficients and thermal shock resistance between the mold base material and any applied surface layer. This mismatch is exacerbated by the abrupt cooling induced by spraying mold release agents. In this context, laser cladding—a form of high-power direct energy deposition (DED)—has gained attention as a surface reinforcement and mold repair technique due to its ability to form metallurgically bonded, wear-resistant coatings with minimal thermal distortion [1-4]. In this study, laser cladding was employed to deposit an 18%Cr–2.5%Ni–Fe stainless steel-based alloy powder (Rockit404) onto SKD61 substrates. The objective was to evaluate its feasibility as a surface coating material to improve thermal fatigue resistance and extend mold life. A diode laser system (Laserline LDF10000-100) with a fiber optic delivery system operating at 900–1,070 nm was used. The system included a 72 mm collimating lens, a 400 mm focusing lens, and a 1,500 μm core diameter laser fiber, producing an 8.3 mm laser spot. The standoff distance between the powder nozzle and the substrate surface was maintained at 20 mm, and argon shielding gas was supplied at 15 L/min. Process parameters, including laser power and powder feed rate, were optimized to ensure stable cladding and uniform deposition. SKD61 specimens (100 × 100 × 25 mm) were prepared by sequential grinding (#320 to #2000 grit) and cleaning with acetone to enhance laser energy absorption. The cladded layers were characterized through cross-sectional microstructural analysis and hardness profiling. Furthermore, erosion resistance was evaluated by immersing the samples in molten ALDC12 aluminum alloy. The laser-cladded Rockit404 coatings demonstrated strong metallurgical bonding, increased surface hardness, and improved corrosion and erosion resistance compared to the uncoated SKD61. These results confirm the potential of SUS-based laser cladding as a viable surface treatment for improving the durability of HPDC molds. The findings contribute to ongoing efforts in developing advanced mold regeneration technologies and surface engineering solutions for the die-casting industry.

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Hot plastic deformation of SLM-printed ZK60 magnesium alloy

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Keywords: activation energy, hot compression test, processing maps, SLM printing, magnesium alloys,

Research into the thermo-plastic processing of magnesium-zinc alloys is an important direction in materials engineering, driven by the increasing demands on modern structural materials. Magnesium alloys are distinguished by their extremely low density, making them among the lightest structural metals available. Combined with the addition of zinc to improve mechanical properties and corrosion resistance, these materials are becoming an attractive alternative to aluminum or titanium alloys in applications requiring weight reduction, such as aerospace, automotive and consumer electronics.

A key challenge in processing these alloys is their limited ductility at low temperatures due to their hexagonal crystallographic lattice, which limits the potential for plastic deformation. Understanding the mechanisms occurring during thermo-plastic processing, such as dynamic recrystallization, dislocation displacement and activation of additional slip systems, allows optimization of processing processes. As a result, the material's forming ability, as well as its final mechanical properties, can be improved.

The development of process maps that describe the relationships between temperature, strain rate and microstructure is key to predicting the behavior of alloys under real processing conditions. These maps make it possible to design more efficient and economical processes for producing components of complex geometries. In addition, the development of knowledge in this field contributes to reducing CO_2 emissions, as lighter materials allow for lower fuel consumption in vehicles.

The evaluation of the coefficient of thermal expansion and the determination of any phase transformations occurring in the solid state were determined according to the scheme shown in Figure 1.

Results and discussion

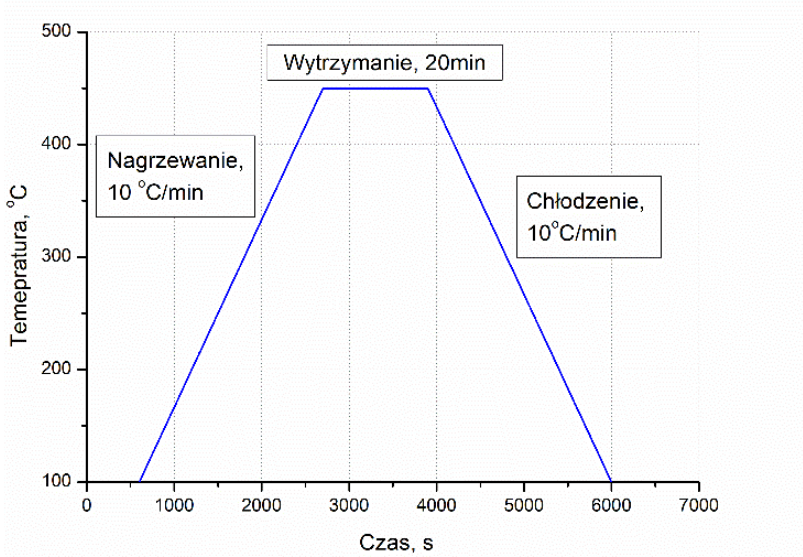


Figure 1: Scheme of thermal analysis for evaluating the coefficient of thermal expansion and detecting possible phase transformations of ZK60 alloy.

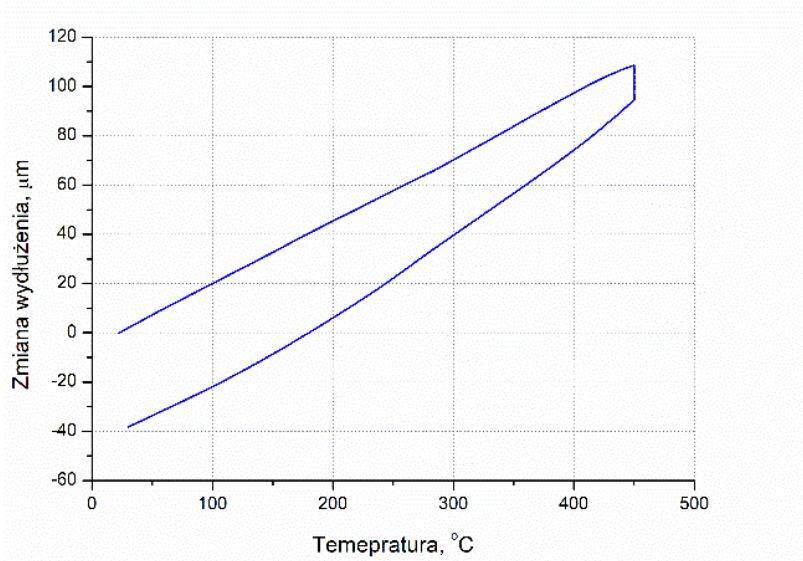


Fig. 2 Change in elongation as a function of temperature

The analyzed alloy in the temperature range up to 450 °C does not show solid state phase transformations.

A diagram of the heat-plastic processing of ZK60 alloys is shown in Figure 3.

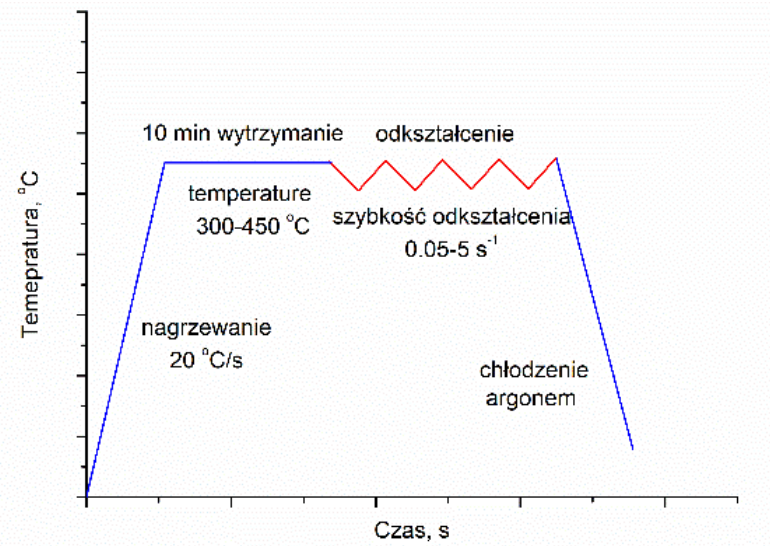
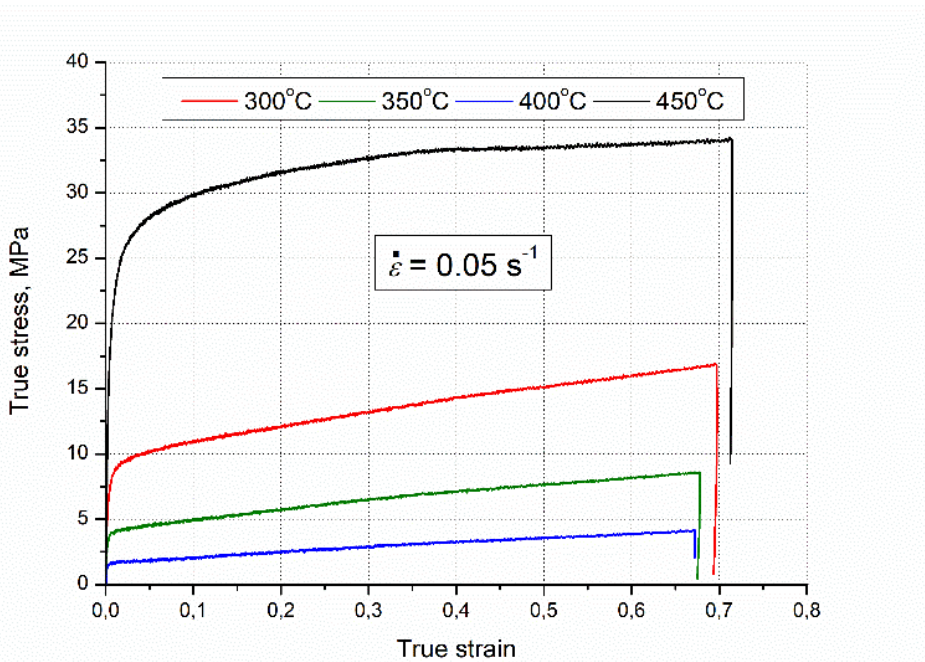
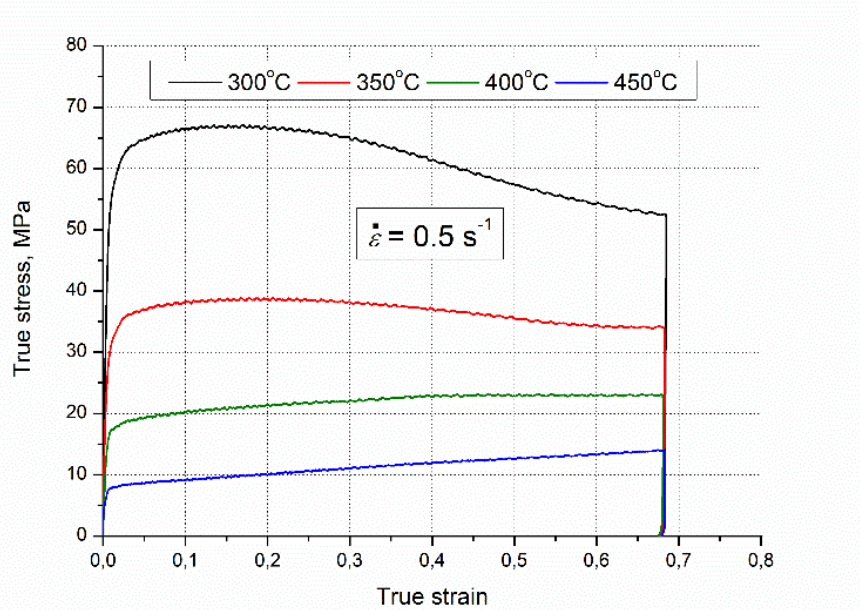


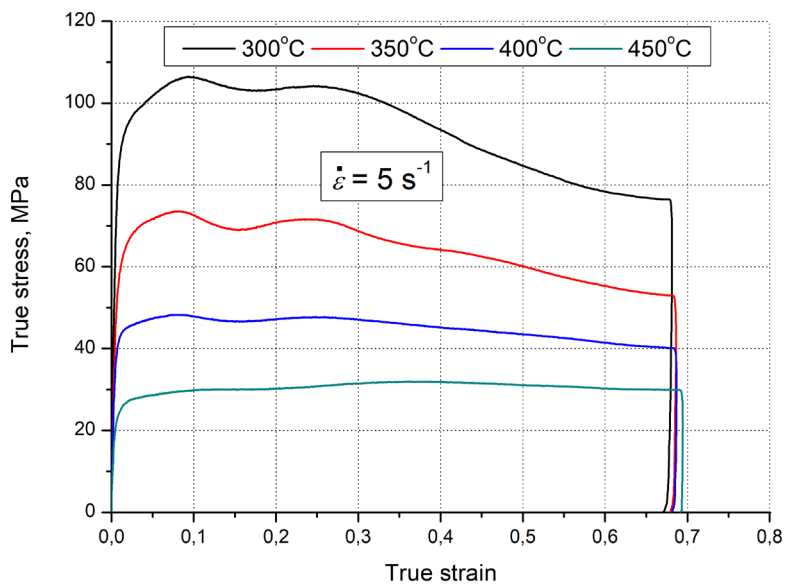
Figure 3: Diagram of the heat-plastic processing of ZK60 alloys.



Rys. 4. Strain stress curves for ZK60 at $\dot{\varepsilon} = 0{,}05\ s^{-1}$



Rys. 5. Strain stress curves for ZK60 at $\dot{\varepsilon} = 0{,}5\ s^{-1}$



Rys. 6. Strain stress curves for ZK60 at $\dot{\varepsilon} = 5\ s^{-1}$

The graphs show the dependence of stress as a function of hot plastic strain of ZK60 alloy. Analyzing their shape, it can be concluded that higher temperature leads to lower melt stress. As the strain temperature increases from 300°C to 450°C, the melt stress decreases. This is because at higher temperatures the material softens due to increased mobility of atoms, reducing resistance to plastic deformation. At 300°C and 350°C, the stress-strain curves show a continuous increase in stress, indicating significant hardening with limited softening. At these temperatures, dynamic recrystallization (DRV) dominates, as the material does not have sufficient energy to effectively initiate dynamic recrystallization (DRX).

At 400°C and 450°C, after an initial peak, the stress decreases, suggesting the occurrence of dynamic recrystallization (DRX). This process produces new, smaller grains, reducing internal stresses and leading to softening.

This effect is more pronounced at 450°C, where DRX is more efficient, leading to a significant decrease in stress.

Increasing the temperature improves ductility and lowers flow stresses, making the material easier to deform. For alloys deformed at 0.05 and 0.5 s-1, the behavior of the material at the analyzed temperatures is identical. For an alloy deformed at 5 s-1, the occurrence of dynamic recrystallization (DRX) occurs for all temperatures, although peak stresses occur at different strain rates.

Regulation mechanism of ni-fe alloy thermodynamic parameter coupling effects on stability enhancement in compressor porous casing systems

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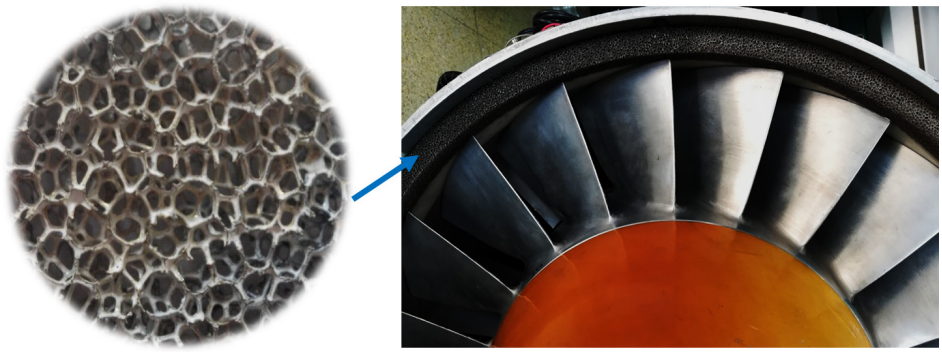
Keywords: Ni-Fe alloy, thermodynamic parameter, compressor, foam metal, casing treatment

Surge and rotating stall constitute fundamental challenges in compressor flow instability, while conventional geometric casing treatments face limitations in operational adaptability. This study proposes a novel approach by leveraging the thermodynamic characteristics of Ni-Fe alloys to optimize the long-term stability of porous casing materials. The investigation initiates with the construction of five Ni-Fe alloys with distinct atomic ratios (Ni_4Fe_{12}, Ni_8Fe_8, $Ni_{10}Fe_6$, $Ni_{12}Fe_4$, and $Ni_{14}Fe_6$) using the special quasi-random structure (SQS) method[1] .First-principles calculations[2] are employed to optimize these configurations and evaluate their thermodynamic properties. Results demonstrate that all alloys exhibit monotonically increasing constant-volume heat capacity with temperature, while the Ni_12Fe_4 configuration displays the lowest overall values. The Debye temperature analysis reveals superior lattice stiffness in $Ni_{12}Fe_4$ compared to other alloys. Thermal expansion coefficient measurements indicate comparable dimensional stability between $Ni_{12}Fe_4$ and Ni_4Fe_{12}/$Ni_{10}Fe_6$ configurations, with enhanced performance over $Ni_{14}Fe_6$. Based on the comprehensive evaluation of thermodynamic stability and flow control performance, the $Ni_{12}Fe_4$ configuration demonstrates optimal suitability for compressor operational conditions. This structural superiority originates from its balanced thermal characteristics that enable effective energy dissipation while maintaining dimensional integrity under aerodynamic-thermal coupling effects. Experimental verification using 70% Ni-content foam metal[3] demonstrates that the foam metal casing treatment (FMCT) achieves a 15.1% improvement in compressor stability margin at Position 4, accompanied by merely 0.56% efficiency loss. The close alignment of characteristic curves suggests minimal impact on steady flow fields, distinguishing FMCT from conventional casing treatments. The power spectral density (PSD) analysis reveals effective suppression of pre-stall disturbances, implying that the energy dissipation mechanism inherent in the material structure inhibits the development of flow instabilities.



Foam metal casing treatment

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Preparation of FeNi alloys with enhanced magnetic properties through High-Speed Linear Heating

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Keywords: ordered $L1_0$-FeNi structure, magnetic properties, high-speed temperature scanner (HSTS)

FeNi alloys have gained significant interest because of their superior magnetic characteristics along with their structural integrity and wide-ranging industrial uses. FeNi alloys have perfect properties for use in magnetic storage devices, transformers, and electromagnetic shielding materials because they have high saturation magnetization and low coercivity as well as excellent corrosion resistance. These alloys serve as essential elements in spintronics and soft magnetic materials where high-performance magnetic materials are required. The ordered $L1_0$-FeNi structure demonstrates high magnetic anisotropy but ordered structure formation faces difficulties because the energy difference between Fe and Ni atoms is minor, which results in slow formation of the ordered phase. Achieving the ordered structure requires extended thermal treatment at 300–400°C for several months which is impractical [1].

Meteorites as extraterrestrial objects demonstrate natural occurrences of FeNi alloys within their composition. Naturally occurring FeNi alloys in meteorites exhibit similar characteristics to their synthetic counterparts while helping researchers understand FeNi alloy behavior under extreme conditions such as space's high temperatures. Research into meteorite compositions has demonstrated that FeNi alloys have proved to be of great interest for applications that demand both high thermal stability and magnetic properties in extreme environments.

The solution in this regard is to add alloying elements to the synthesis process (such as boron (B), aluminum (Al) and silicon (Si)). The added elements promote the formation of the ordered structure and either strengthen or maintain the magnetic moment. The addition of B into alloys results in lattice strain which increases both their strength and magnetic properties. The elements aluminum and silicon facilitate the order formation process which reduces the processing time and enables an increase of the magnetic moment. In addition, introducing of B, Al and Si in the alloy increases its thermal stability, making it more resistant to degradation during high-temperature processing [2].

Given the problems associated with traditional synthesis methods, the synthesis of ordered FeNi based alloys under programmed heating conditions was proposed. This involves high-speed linear heating using a High-Speed Temperature Scanner (HSTS-3) technique [3]. The latter leads to a faster formation of the ordered structure, significantly reducing the need for long-term heat treatment. It allows to select the necessary temperature conditions for the synthesis of the material at various heating rates (up to 10000 °/min), while simultaneously allowing to study the microstructural changes and XRD patterns that occur during heating and subsequent fast cooling, as well as characterize magnetic properties.

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Phases evolution in the annealed $Ni_{50}Mn_{20}Sn_{30}$ Heusler alloy obtained by mechanosynthesis

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Keywords: Heusler alloys, mechanosynthesis, annealing, electrical resistivity

Ni-Mn-Sn alloys are part of the Heusler alloy family, having the L_{21} crystallographic structure with the formal composition X_2YZ [1]. The highest properties of the Heusler alloy are obtained if the crystallographic order is as high as possible. If the compositions are slightly modified new properties are expressed, namely a martensite transition occurs [2]. However, the obtaining of the alloy by arc melting requires long and high temperature annealing times and this research propose a nonconventional way of alloy obtaining: mechanosynthesis. In this way the aspect of the nanostructure is introduced as well as the internal stresses with high impact on structure and properties [3].

As composition, the Ni50Mn20Sn30 alloy is proposed to be obtained by mechanosynthesis in high energy ball milling. The elemental powders were milled up to 10 h and after this time frame a disordered B_2 structure was obtained. To modify the crystal structure, annealing at temperatures up to 700 °C was performed. As the temperature increases, the internal stresses were removed and gradually the L_{21} structure appears as the temperature increases above 350 °C. At the final temperature (700 °C) small amounts of parasite phases were visible (NiMnSn and Ni_3Sn). Using Rietveld analysis, it was found a L_{21} phase is obtained in the sample volume up to 95 %. During the annealing process, the internal stresses, mean crystallite size, were computed. The morphology and composition changes were analysed by scanning electron microscopy and energy dispersive X-ray spectroscopy. The influence of the phase change versus temperature was analysed by measuring the magnetic and electrical resistivity response of the samples.

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Continuous annealing of medium-Mn steels: thermal characterization and optimalization process of heat treatment

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Keywords: medium-Mn steel, continuous annealing, sustainable manufacturing, rapid optimization, dilatometry, heating rate

The conventional manufacturing process for medium-Mn sheet steels, including intercritical processing, typically involves multi-hour batch annealing, which has poor environmental and economic efficiency. Additionally, this process leads to significant variability in the steel's mechanical properties depending on the coil position, resulting in material waste. Consequently, it is unsuitable for producing high-quality automotive body components. There is a research gap and an industrial demand for a more sustainable, cost- and time-efficient large-scale production method that can be implemented using existing facilities.

To address this, a continuous-annealing process with a soaking time of less than 120 seconds was developed and optimized for medium-Mn steel. The study established heating conditions compatible with conventional electric furnaces. To streamline and accelerate the optimization of temperature-time parameters for mechanical properties, a novel "rapid optimization" method using a dilatometer was introduced. This approach enables precise, time-efficient, and waste-reducing heat treatment optimization for newly designed steels.

The findings demonstrated the feasibility of applying continuous annealing to the heat treatment of advanced medium-Mn steel. Minor adjustments to thermal parameters enabled the formation of lath-like microstructures with varying thickness and retained austenite stability, allowing broad control over both strength (YS, UTS) and ductility (TEl), achieving a UTS × TEl threshold of 37 GPa%. These results indicate the potential for implementing the proposed heat treatment conditions in industrial steel production for diverse applications.

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Comparative study of heat treatment effects on the microstructure and mechanical properties of lpbf-processed AlSi7, AlSi10mg and AlSi12 alloys

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Keywords: LPBF, aluminium, heat treatment, microstructure

This study investigates the microstructural evolution of AlSi7, AlSi10Mg, and AlSi12 alloys fabricated via laser powder bed fusion (LPBF) under various heat treatment regimes. The resulting microstructures were characterized using scanning electron microscopy (SEM) and electron backscatter diffraction (EBSD) to analyze phase transformations, particle size evolution, and recrystallization (REX) behavior. Quantitative analysis of particle size distribution was performed to track the coarsening kinetics. The influence of heat treatment on the mechanical properties was evaluated through compression testing. Results demonstrate significant variations in microstructural development across the three alloys, with distinct responses to the applied thermal treatments, including changes in phase transformations. This comparative analysis provides valuable insights into tailoring the microstructure and mechanical performance of LPBF-processed AlSi alloys through controlled heat treatment.

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Laser welding of Ni-coated mild steel tabs to 18650 lithium-ion battery cells using a diode laser system

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Keywords: lithium-ion battery, 18650 cell, diode laser welding, Ni-coating, welding parameter optimization, mechanical strength, energy storage

This study reports on the laser welding of nickel-coated mild steel to 18650-type lithium-ion battery cells using a diode laser system, with a focus on the mechanical and structural characteristics of the joints formed on the positive terminals of the cells. In electric vehicle battery packs—typically composed of hundreds or thousands of individual cells—long-term reliability largely depends on the quality of the electrical and mechanical connections. Therefore, developing a welding process that ensures high mechanical strength, good electrical conductivity, and stable microstructure is essential.

Commercially available Ni-coated mild steel (DC01) sheets were selected as the interconnecting tab material to ensure compatibility and weldability with the battery terminals using a 400 W diode laser. Both the positive and negative terminals of the cylindrical 18650 cells were made of the same material as the tab. The thicknesses of the positive and negative terminals were 0.5 mm, and the tab thickness was 0.2 mm.

The laser welding process was carried out using a Coherent Dilas Compact Evolution diode laser system with a maximum output of 500 W and a wavelength of 960 nm. The experimental setup focused on two main process parameters: laser power and welding time. Weld quality was evaluated by tensile testing of the joints, and metallographic cross-sections were prepared for microstructural analysis. The goal was to determine the optimal parameters that produce strong, reliable welds without damaging the battery cells.

It was observed that excessive heat input—either due to long exposure times or high power levels—can damage the battery casing and pose an explosion risk due to internal pressure buildup and potential thermal runaway. The research successfully identified safe parameter ranges that produce high-quality welds with good mechanical integrity and microstructural consistency.

This work contributes to the development of advanced manufacturing processes for high-energy-density, modular battery systems, particularly in the electric vehicle industry, where durable and reliable connections are critical for overall system performance and lifespan.

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T17: Nanofluids

Optimization of nanofluid concentration and flow rate in evacuated tube solar collectors using anova: energy and exergy analysis

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Keywords: nanofluids, evacuated tube solar collector, ANOVA, energy efficiency, exergy analysis, MWCNT

This study experimentally investigates the impact of multi-walled carbon nanotube (MWCNT)/water nanofluid concentration and flow rate on the thermal performance of an evacuated tube solar collector (ETSC). Nanofluids with weight fractions of 0.005%, 0.01%, and 0.05% MWCNT were tested under six flow rates (1–3.5 L/min) to evaluate energy efficiency, exergy efficiency, and entropy generation. A two-step preparation method ensured nanofluid stability, while ASHRAE Standard 93-2003 guided thermal performance evaluations. Statistical analysis via ANOVA was employed to identify significant factors and optimise parameters. Results demonstrated that increasing nanofluid concentration and flow rate enhanced both energy and exergy efficiencies. The 0.05% MWCNT nanofluid at 3.5 L/min achieved peak energy efficiency (59%) and exergy efficiency (11.5%), surpassing distilled water by 16.1%. ANOVA revealed that concentration had the most pronounced effect on efficiency, while flow rate significantly influenced heat removal factors and entropy minimization. The overall heat loss coefficient decreased by 27% for nanofluids compared to water, highlighting improved thermal management. This work provides data-driven insights into optimising nanofluid-enhanced ETSCs, emphasising the synergy between concentration and flow rate for maximising solar thermal efficiency. The findings advance the application of nanofluids in renewable energy systems, offering a pathway to reduce collector size and operational costs while improving sustainability.

The effect of dopants on the thermal conductivity of zinc oxide nanofluids

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Keywords: ZnO, nanofluids, thermal conductivity, FTIR

Nanofluids have novel properties that make them useful in applications in heat transfer, including microelectronics, batteries and fuel cells. The nanofluids are colloidal suspensions of nanoparticles (oxide, metal) in a base fluid (water, oil). Zinc oxide is a non-toxic oxide with high thermal conductivity and high refractive index, properties that recommend it for obtaining nanofluids with efficient heat transfer.

In this work, doped zinc oxide nanoparticles as well as nanofluids with enhanced heat transfer were synthesized and characterized. As is known, doping leads to changes in the structure and morphology of zinc oxide. Zinc oxide was doped with silver and nickel ions and their influence on the structure, morphology and properties of the obtained nanoparticles and nanofluids was investigated.

Doped zinc oxide solutions were obtained by sol-gel method. Gels were characterized by DTA/TG in order to establish the heat treatment temperature and by FTIR spectroscopy to analyse their structures. TG curves show the elimination of all organic residues below 400°C and crystallization effect between 430°C and 455°C depending on the dopant used.

Nanoparticles obtained after heat treatment at 500°C were characterized by FTIR to identify structural groups and XRF to obtain their chemical composition. The FTIR spectra of the nanoparticles show a shift in the position of the Zn-O- band, showing the influence of dopants on the structure of zinc oxide. Crystalline phases of nanoparticles were identified by X-Ray Diffraction. The morphology of the nanoparticles was studied by Transmission Electron Microscopy.

After characterizing the particles, the nanofluids were prepared. Water was chosen as the base-fluid due to its beneficial properties, such as naturally high thermal conductivity, low viscosity, and low cost. According to zeta potential tests, the doped nanoparticles form more stable dispersions in deionized water than the undoped ZnO nanoparticles. This suggests that even a few percent of foreign material can change the structure of ZnO to produce a more stable dispersion.

Several different surfactants were tested to achieve sufficiently stable dispersions with all four types of particles. The best stability was achieved using Gum Arabic. Viscosity tests revealed that the surfactant causes a greater increase in viscosity than the particles themselves. To avoid this unnecessary increase, the effect of the surfactant amount on the stability of the dispersion was investigated. Way less than 10 mass% of the solid particles is enough. During the dispersion process, a reasonably good suspension was achieved. The concentration of these stable dispersions was determined by drying small samples of the nanofluids. The stable dispersions were then diluted to a 0.2 v/v% particle concentration. The particles caused a 2.4–2.9% increase in thermal conductivity compared to the base fluid at room temperature. The surfactant had no measurable effect on thermal conductivity, so the thermal conductivity of the base fluid can essentially be considered that of pure water.

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T18: Nanomaterials and composites

Thermal analysis as a successful tool for the nanocomposites development: influence of copper oxide nanoparticles on the bulk polymerization of diaminomaleonitrile

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Keywords: diaminomaleonitrile, CuO, bulk polymerization, DSC, nanocomposite

In recent years, our research has concentrated on utilising the diaminomaleonitrile (DAMN) as a monomer to synthesise conjugated polymers featuring C=N bonds [1,2]. The primary objective has been to establish simple, cost-effective, and environmentally friendly methods for producing these multifunctional materials. DAMN-based polymers have gained significant attention, with studies exploring their synthesis, optical and electromagnetic properties [1,2], and diverse applications across chemistry, physics and biology [3]. In this context, thermal analysis techniques have proven to be powerful tools for optimising the synthetic conditions of DAMN polymerisation, as well as for elucidating the kinetics and pathways of these highly efficient reactions [4,5]. A further step in the development of new materials has been the functionalisation of these polymers based on DAMN, a crucial aspect for enhancing performance in various applications, such as catalysts, electronic displays or nanoparticle biosensors. Thus, to address this challenge, this study investigates the impact of CuO nanoparticles on the bulk thermal polymerisation of DAMN under different temperature regimes, in accordance with the solid-state and melt polymerisation of this unique dinitriles monomer. The process was effectively monitored using differential scanning calorimetry (DSC), as described in previous studies [4,5]. Herein, it is demonstrated that CuO exerts a pronounced effect on the polymerisation reaction, possibly due to a coordination process occurring between Cu^{2+} and the amino and/or cyano groups of DAMN, as detected by DSC and Fourier transform infrared (FTIR) spectroscopy. Additionally, thermogravimetric (TG) and *in situ* mass spectrometry (MS) measurements enabled the analysis of gases evolved during the thermal-induced transformations of DAMN in the presence of CuO, providing new insights into the polymerisation mechanism of this monomer. Moreover, this thermal study supported the efficient preparative-scale synthesis of CuO-DAMN-based nanocomposites with potential applications in (photo)catalysis. So, as an initial approach to them, these novel composites were successfully tested by DSC as an additive in the thermal decomposition of ammonium perchlorate, offering promising prospects in solid propulsion aerospace technology.

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A novel facile synthesis of cmk-type carbon replicas Cast from narrow-mesoporous silica matrices

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Keywords: CMK-1, CMK-2, MCM-48, SBA-1, carbon replica

Nanoreplication, which relies on the casting of mesostructured carbons (replicas) with ordered porosity from mesoporous silica materials (templates), was reported for the first time in 1999 by Ryoo et al. [1,2]. Carbon replicas featuring the characteristics of molecular sieves are a family of materials that in many respects reveal properties superior to those of classic activated carbons. First of all, although they are built of disordered carbonaceous matter, they possess a long-range spatial ordering of the pore network, being in fact a negative structure of the mineral template used. Thus, unlike conventional microporous activated carbons, mesostructured carbons are essentially mesoporous bodies. Moreover, carbon replicas reveal well developed and adjustable textural parameters, chemical inertness, and good (hydro)thermal stability accompanied by a tuneable surface composition and interesting electric properties. With such beneficial characteristics, they found plenty of applications in various fields, i.e., adsorption/separation science, catalysis, medical purposes, and electrochemical device design. Nevertheless, despite their excellent properties, research on the practical applications of mesostructured carbons did not cross the laboratory threshold. This is due to the tedious, multistep, and energy-consuming procedures of their synthesis, including the preparation of a suitable silica template followed by incorporation of the carbon source (originally, incipient wetness impregnation with aqueous sucrose solution), carbonization of the composite, and, finally, leaching of the mineral template. Among these steps, deposition of the carbon source is of paramount importance in view of the quality of the ultimate replica (structural ordering and textural features).

In this work, we developed a new facile and versatile procedure for the synthesis of two carbon replicas, namely CMK-1, and CMK-2, cast from narrow-mesoporous ordered silicas, i.e., MCM-48 and SBA-1, respectively [3]. The recipe relies on spontaneous precipitation polycondensation of a carbon precursor (furfuryl alcohol) on a silica template in an aprotic solvent (toluene). This process is driven by the adsorptive interaction of polar monomer molecules with free silanol groups on the silica surface, which provides even coverage of the entire porous structure of the matrix with the carbon precursor. This in turn leads to the formation of exact negative carbon structures with excellent long-range order of the porous structure as well as exquisitely developed specific surface area and high total pore volume. Furthermore, the original particle morphology is preserved. The scalability and repeatability of the synthesis were also proven. We believe that the proposed synthesis pathway opens the way to the applicability of carbon replicas on a technological scale.

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Material analysis of newly developed resin-based multilayer composites

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Keywords: differential scanning calorimetry, activation energy, cure, laminate, modified epoxy resin

Over the last decades or so, the automotive industry has seen an increase in the use of composite materials. These materials are characterized by their relatively low density and, at the same time, high mechanical strength. In addition, they can be easily formed, even though they are highly rigid. The research aimed to prepare an ultralight multilayer composite material (laminate) dedicated to racing vehicle shells. The composition of the matrix is fundamental in a laminate, which has a bearing on the weight of the resulting composite and its final properties. Preliminary research into the development of a suitable resin composition for the matrix of a multilayer composite material was carried out, with a total of 44 laminates produced, differing in the composition of the resin, the number of layers, and the manufacturing process. In this research, a number of different matrix compositions based on epoxy resins of the Epidian 5 (EP5) and Epidian 6 (EP6) type, modified with an active solvent (n-butyl glycidyl ether) and cured at room temperature with different types of hardeners, were made. Laminates were also made using commercially available mixtures of ready-to-use systems based on EP5 or EP6. All the variants prepared were tested mechanically to determine the best compositions and the most suitable manufacturing process. The study focused on assessing the influence of the matrix composition on the strength properties of the multilayer composite material. Hardness, impact strength, and three-point bending tests were performed, and the densities of the developed resin compositions and laminates were determined.

In addition, differential scanning calorimetry (DSC) analysis was used to characterize the curing reaction of the matrix and the final property of laminates. This method can provide information about glass transition temperature (Tg), onset of cure, heat of cure, maximum rate of cure, completion of cure, and degree of cure of material. The DSC method was a valuable tool for adequately describing the experimental cure kinetics. The activation energy of the curing reactions in a dynamic mode was obtained using Kissinger and Ozawa methods. Investigating the curing process of different matrix systems using DSC can be a useful tool that, in a less costly way by using less material, allows the most promising systems to be pre-selected for further experiments in the production of laminates. In addition, as already mentioned, it is possible to control the degree of curing of the obtained laminates, which is one of the important parameters of the achieved material. Thermal characterization studies on

thermosetting resin materials could help avoid production problems, choose the system for producing laminates, and troubleshoot already at the stage of preparing the composition. This knowledge is invaluable and will help reduce material consumption, which will translate into environmental protection and sustainable production.

Green synthesis of copper oxide nanoparticles using peppermint leaf extract: characterization and antimicrobial activity

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Keywords: CuO, nanoparticles, green synthesis, peppermint leaf, antimicrobial

Green synthesis using plant extracts has recently gained significant attention due to its cost-effectiveness, feasibility, and environmentally friendly nature. In this study, copper oxide nanoparticles (CuO NPs) using peppermint leaf extract as a natural reducing and stabilizing agent have been synthesized. The obtained nanoparticles were characterized using several techniques, including UV-visible spectroscopy, X-ray diffraction (XRD), Fourier-transform infrared (FTIR) spectroscopy, and scanning electron microscopy (SEM). XRD analysis revealed a monoclinic crystal structure with an average crystallite size of 5 nm, as determined by the Scherrer equation. The thermal properties of the CuO NPs were examined using thermogravimetric and differential thermal analysis (TG/DTA). The synthesized nanoparticles exhibited promising antimicrobial activity.

Acknowledgments
The research was funded by the Executive Agency for Higher Education, Research, Development and Innovation Funding (UEFISCDI), grant number PN-IV-P7-7.1-PED-2024-0582, no. 21 PED/2025.

Photocatalytic degradation of Methylene Blue (MB) and Rhodamine 6G (Rh 6G) using g-C_3N_4/TiO_2 composites synthesized by hydrothermal method

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Keywords: photocatalysis, g-C_3N_4, TiO_2, hydrothermal synthesis, Methylene Blue, Rhodamine 6G, wastewater treatment

In this study, graphitic carbon nitride (g-C_3N_4) and titanium dioxide (TiO_2 composites were synthesized by hydrothermal method and applied as photocatalysts for the degradation of organic dyes: Methylene Blue (MB) and Rhodamine 6G (Rh 6G). The work aims to enhance UV-Visible light-driven photocatalytic activity by combining the advantageous properties of both g-C_3N_4, a with a narrow bandgap, and TiO_2, a well-known but UV-active photocatalyst. The synthesized g-C_3N_4/TiO_2 composites were characterized using Thermogravimetric analysis (TG), X-ray diffraction (XRD), scanning electron microscopy (SEM), Electron diffraction spectroscopy (EDX), Photoluminescence (PL) and UV-Vis diffuse reflectance spectroscopy (DRS) to investigate their structural, morphological, and optical properties.

The TGA curve under air conditions shows a sharp decomposition of g-C_3N_4 between 500–650 °C, leaving only ~1.4% residue, indicating nearly complete oxidative degradation. Whereas under nitrogen atmosphere, a similar weight loss occurs in the same temperature range, but a higher residue of ~9.9% remains, suggesting partial carbonization and greater thermal stability in inert conditions. TiO_2 is not thermo degradable because of its thermodynamically stable and very high temperature needed as compared to the graphitic carbon nitride.

Results indicated successful integration of TiO_2 with g-C_3N_4, leading to improved light absorption in the visible region and enhanced charge separation efficiency.

Photocatalytic performance was evaluated under UV-visible-light irradiation, and the degradation efficiency of MB and Rh 6G was monitored using UV-Vis spectrophotometry. The composite photocatalysts demonstrated significantly higher degradation rates compared to pure TiO_2 or g-C_3N_4 a lone. Among the tested samples, the optimal g-C_3N_4/TiO_2 ratio exhibited 95% for MB and 96% for Rh 6G degradation within 180 min of light radiation.

The enhanced performance is attributed to the synergistic effect between g-C_3N_4 and TiO_2, where the heterojunction facilitates charge transfer and suppresses electron-hole recombination. This work highlights the potential of g-C_3N_4/TiO_2 composites as enhanced, efficient, low-cost photocatalysts for the treatment of dye-contaminated wastewater and offers insights into the rational design of visible-light-active photocatalytic materials.

Acknowledgments
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Silica-based coatings of cellulose substrates for improved flame retardancy properties

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Keywords: silica-based coatings, cellulose substrate, flame retardancy properties

Halogens, typically found in conventional flame retardants (FRs), have the potential to emit harmful gases during fire incidents. Consequently, there is a growing interest in developing halogen-free flame retardants that are safer for human health and the environment during fire incidents.

In this study, environmentally friendly and cost-effective copper (Cu)-containing silica-based coatings were developed and evaluated for their flame-retardant properties and deposited on cotton fabrics. Cu-containing silica solutions with and without polyvinyl alcohol (PVA) were prepared using the sol-gel method and applied through immersion on the cotton fabric, followed by drying at 80 °C and curing at 170 °C. The influence of PVA on the flame retardancy ability of the resulting coatings was evaluated. Thermal analysis (TA), attenuated total reflectance infrared spectroscopy (ATR-IR), X-ray diffraction (XRD), and scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM-EDS) were employed to evaluate the structure, morphology, and thermal behaviour of the coated samples. TA results revealed significant improvements in thermal stability for Cu-doped silica-coated cellulose compared to uncoated substrates. SEM imaging demonstrated a uniform and continuous coating over the cellulose substrate surface. Vertical flame resistance (VFT) test showed that the Cu-doped silica coatings enhanced the fire resistance of the cellulosic substrates. Notably, differences in flame retardancy were observed between coatings formulated with PVA and those without it, indicating that PVA has an influence on improving coating performance

Acknowledgments
The research was funded by the Executive Agency for Higher Education, Research, Development and Innovation Funding (UEFISCDI), grant number PN-IV-P7-7.1-PED-2024-0582, no. 21 PED/2025.

Thermal treatment and polymer matrix diffusion effects on hydroxyapatite particle size evolution

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A widely used approach for synthesizing hydroxyapatite (HA) particles is the wet chemical precipitation method, favored for its cost-effectiveness and straightforward process [1]. Incorporating organic macromolecules with polar functional groups, such as COOH and OH, during synthesis can significantly impact the properties of the resulting HA particles. These functional groups enhance the affinity for positively charged Ca^{2+} ions, promoting HA crystal nucleation in the solution. [2] [3].

In this study, solutions at different concentrations of chitosan and sodium alginate were used as nucleation medium for the HA particles. The calcium and phosphate precursor solutions were firstly adjusted at a pH of 12 and added to the polymer solution with a concentration varying from 5 to 10 % w/v, reported to the stoichiometric mass of HA according to the synthesis reaction. After synthesis, the resulted powder was calcinated at 1000˚C.

The effects that the polymers have on the properties of HA particles were monitored by means of SEM, FT-IR, EDX, DLS and TGA, before and after the thermal treatment in order to see how the system evolves till crystallisation of HA occurs. The largest decrease in the average particle diameter is 67.7% in the case of the HA+ Alg 10% sample, but a reduction in particle diameter is observed in all samples.

Table 1. Particle size diameter of the sample by DLS

	Temperature	
Sample	**120 ˚C**	**1000 ˚C**
HA	d= 2649 nm	d= 2309 nm
HA+ Alg 5%	d= 1360 nm	d= 728 nm
HA+ Alg 10%	d= 2180 nm	d= 704 nm
HA+ Chit 5%	d= 1421 nm	d= 1186 nm
HA+ Chit 10%	d= 2181 nm	d= 1801 nm

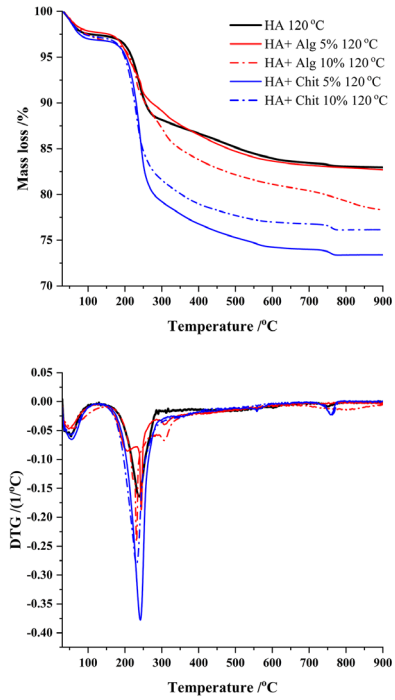

Fig. 1. TG/DTG curves of the samples

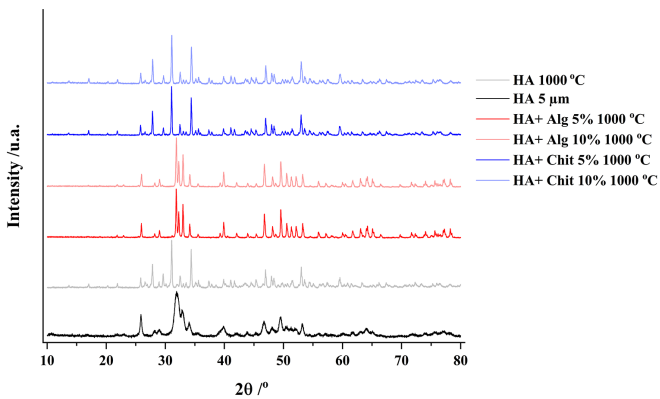

Fig. 2. XRD pattern of the samples

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Fabrication of fibrous nanofiber membranes for passive radiation cooling

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Keywords: passive radiation cooling, nanofiber, silicon dioxide, polyvinylidene fluoride

Passive radiation cooling technology reflects sunlight and emits infrared thermal radiation into the cold outer space through the transparent window of the atmosphere (8–13 μm) without consuming any energy to cool objects. Therefore, it has potential application prospects in many fields and has attracted the wide attention of researchers. In recent years, photonic radiators and metamaterials have been studied in passive radiative cooling. However, they are usually not flexible, low ductility, complex shape and demand a high level of precision, which severely restricts large-scale manufacturing and limits their practical application. A simple and high-efficient electrospinning method with inexpensive raw materials is demonstrated for fabricating a high-performance fibrous and stretchable polymer nanofiber for daytime passive radiation cooling that consists of polyvinylidene fluoride and polydisperse silicon dioxide (SiO_2) microspheres. For effective scattering by nanofiber structures and silica microspheres, the membrane exhibits an average solar reflectivity of 92.3%. The molecular vibration of polyvinylidene fluoride and phonon polarization resonance of silica microspheres result in an average atmospheric window transmissivity of 0.86. The daytime cooling performance has experimentally demonstrated a maximum temperature decrease up to 5.8 °C under an average solar intensity of 700.8 W/m^2. This work provides a promising method for the scale-up production of radiative coolers with high performance.

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Development of graphitic carbon nitride/metakaolin composite photocatalysts

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Keywords: kaolin, graphitic carbon nitride, composite photocatalyst, solar irradiation

Heterogeneous photocatalysis can be used to remove many environmental pollutants. Their application is particularly promising in environmental technologies to satisfy both green chemistry and efficient degradation requirements. A current aim is to synthesize photocatalysts with enhanced ability to harvest natural sunlight, and therefore to establish their more viable practical application. Graphitic carbon nitride (g-CNx) is a non-toxic, environmentally friendly *n*-type semiconductor has a band-gap of ca. 2.7 eV (459 nm), however it usually has fast recombination of photoinduced electrons and holes, low quantum efficiency, low specific surface area and poor quantum yield. The disadvantages can be balanced by composite synthesis and the appropriate selection of precursor, such as urea [1]. Kaolin is an abundant, natural and cheap raw material, used in many industrial applications. Photochemically active graphitic carbon nitride can be in-situ synthesized onto the surface of a clay minerals, significantly improving their catalytic properties. The elevated temperatures (usually T>350°C) could induce structural alterations (i.e. dehydroxylation) of the 1:1 type phylloalumonosilicate framework [2].

In our work, graphitic carbon nitride/metakaolin composite photocatalysts were synthesized from urea precursor. The effect of the annealing temperature and the synthesis efficiency in the presence of kaolin were investigated. Structural characterization by X-ray diffraction (XRD) and infrared spectroscopy (FTIR) verified the successful, in-situ thermal polycondensation of nitrogen-rich g-CNx along the thermal dehydroxylation of kaolinite to metakaolin at 450-550°C range. The thermal stability and the g-CNx content of the composites were determined by thermal analysis (TG-DTG) and CHN analysis, and found to be ranging from ca. 87 m/m% to ca. 2 m/m%. The specific surface area (BET-SSA) was determined by nitrogen adsorption, which showed an increased after composite synthesis to 67–89 m^2/g. The presence of kaolin during the thermal synthesis was found to have a significant effect: the yield of in-situ formed g-CNx drastically decreased (from ca. 4.9 m/m% to 3.8–0.1 m/m%) with increasing kaolin content. Optical band gaps were determined by UV-Vis-DRIFT and indicated the affinity to absorb part of the visible-light ($\lambda < 413$ nm). Photo-induced catalytic activity upon both UV and artificial solar irradiation was observed by hydroxyl radical evolution using a coumarin radical scavenger compound. Our results indicates that the application of metakaolin-based g-CNx composite photocatalysts could be promising.

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T19: Organic materials

Thermal and spectroscopical analysis of new synthesized iron(ii) complexes with glyoximes, schiff bases, semi- and thiosemicarbazones

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Keywords: azomethines, iron complexes, thermo-gravimetric study, spectroscopic study, biological activity

Iron(II) complexes with glyoximes results in the formation of macrobicyclic ligand systems under mild conditions with high yields [1]. Generally, iron compounds are widely used, especially in pharmaceutics and nanotechnology. The use of nanoparticles in medicine as antibacterial agents can be beneficial due to their size, being much smaller than that of bacteria with range of micrometres, or more precisely, the nanoparticles with right size are able to penetrate through pores of their cell membrane. The use of iron complexes as antibacterial agents which contain N- and O-donor ligands are also advantageous because they show stronger antibacterial effect against both Gram-positive and Gram-negative bacteria than the free ligands themselves [2].

In our research project new Fe(II) complexes were synthesized from the reaction between azomethine derivatives (glyoximes, Schiff bases semi- and thiosemicarbazones) and $FeSO_4$ salt, under inert atmosphere in suitable solvent. After presenting a short historical survey, classification, and possible application fields of these compounds, we report the study of their thermoanalytical behaviour (TG-DTG-DTA), spectroscopic features (such as FTIR, Mössbauer, UV-VIS, Raman spectroscopy, mass spectrometry) as well as their powder XRD and AFM or SEM investigations. The biological activity of complexes, especially their antibacterial activity, will also be discussed. A few representative examples for their thermal decomposition are shown in Figure 1.

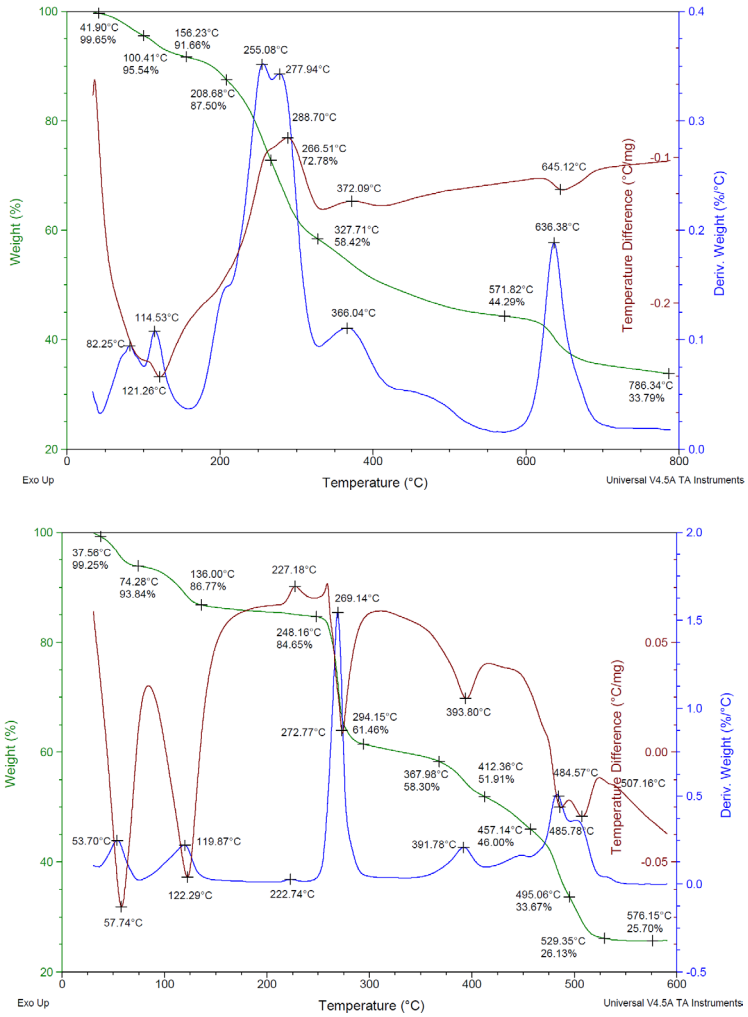

Fig. 1. Thermal decomposition of $[Fe(Ph\text{-}Me\text{-}Diox)_3(BOMe)_2]$ and $[Fe(4\text{-}methyl\text{-}2\text{-}pentanone\text{-}SC)_2]$.

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T20: Pharmaceuticals

Thermoanalytical and spectroscopic study of flunarizine dihydrochloride and binary mixtures of drug and excipients stored in extreme environments

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Keywords: flunarizine dihydrochloride, extreme temperature, thermal analysis, binary mixture, FTIR-UATR spectroscopy

The quality and efficacy of pharmaceutical formulations involves a series of complex processes that require scientific knowledge and time to develop. Any change observed after the manufacture of a pharmaceutical product that affects its suitability or quality is an important factor for the pharmaceutical industry and research.

The dosage form and its composition, the properties of the packaging material, the physical and chemical properties of the biological active ingredient and the pharmaceutical ingredients, as well as environmental factors such as light, temperature and humidity influence the stability of pharmaceutical products [1].

Flunarizine dihydrochloride (Flu), with the molecular formula $C_{26}H_{26}N_2F_2 \cdot 2HCl$, is used as a sedative and for peripheral vascular disorders and cerebral disorders [2].

Most drugs must to be stored at 8 ^{0}C to about 25 ^{0}C as the pharmaceutical formulations are manufactured for this temperature range. Extreme temperatures lead to degradation of many drugs and affect the compatibility of the pharmaceutical components and stability. Little information on this situation can be found in the literature [3]. Accordingly, the aim of our study is to determine the compatibility between the active pharmaceutical ingredient, Flu, and the pharmaceutical excipients after the binary mixtures have been stored at extreme temperatures, exposed to heat and could stress.

The thermal behaviour of Flu stored at ambient and extreme temperatures was analysed by TG/DTG/HF analysis and the compatibility studies with different pharmaceutical excipients were evaluated by TG/DTG/HF, FTIR spectroscopy and high performance liquid chromatography (HPLC) for binary mixtures FLU:excipients = 1:1 (w/w).

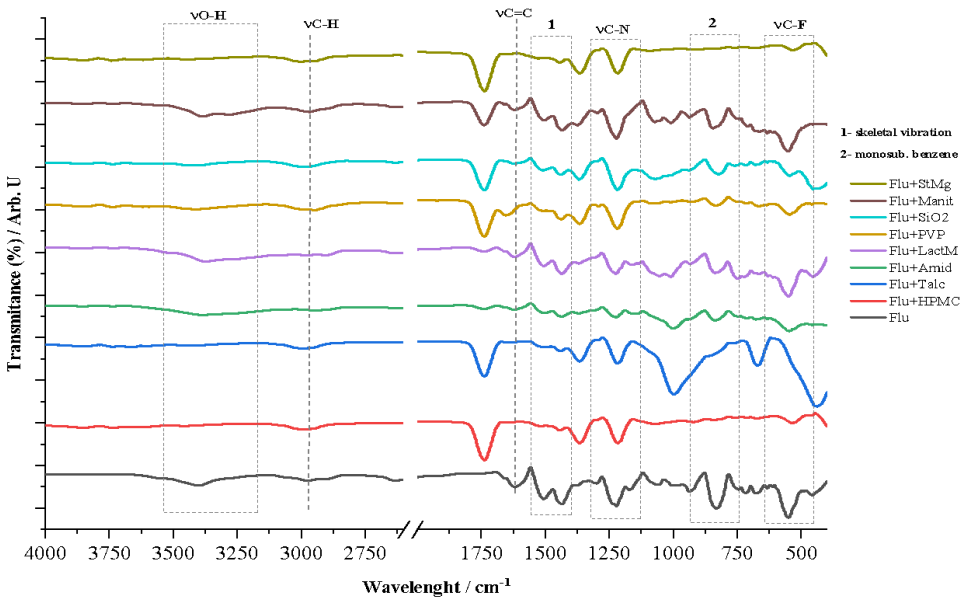

Fig.1 FTIR-UATR spectra of binary mixtures-Flu

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Preformulation studies for antipyretic and analgesic drug in novel pharmaceutical formulation

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Keywords: thermal analysis, FTIR, compatibility studies, alginate, kappa-carrageenan, gelatin

Preformulation studies are essential in the development of new pharmaceutical formulations. A thorough understanding of the physicochemical properties of drugs and pharmaceutical ingredients is crucial for successful optimization of new formulations [1,2]. Tablets are among the most commonly used medication forms due to their safety and efficacy [3].

The aim of our study is to develop new pharmaceutical formulation containing propyphenazone, caffeine and theobromine which is expected to enable faster drug delivery and absorption. Propyphenazone, a derivative of pyrazolone known for its anti-inflammatory, analgesic, and antipyretic effects, is commonly available in tablet form [4].

In this study, sodium alginate, kappa-carrageenan and gelatin were used to prepare hydrogels to investigate the release of the active ingredient at different stages of ingestion. A major focus of the study was to investigate the interactions between the hydrogel components and to assess how the individual preparation steps affect the stability of the material.

The newly obtained dosage form was evaluated using FTIR, thermogravimetric analysis, electron microscopy SEM coupled with EDX and UV-Vis.

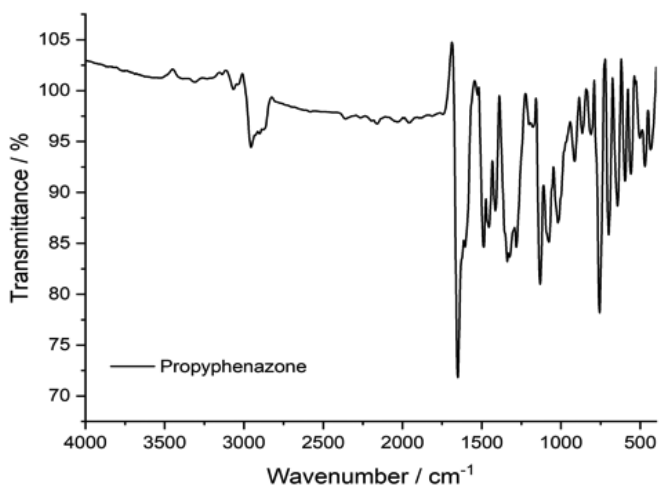

Fig. 1 FTIR spectrum of propyphenazone

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T21: Polymers

Influence of low molecular blocking agent on the structure and thermal properties of modified bio-based triisocyanates

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Keywords: blocked isocyanates, blocking agent, isocyanates modification, sustainable production

Polymers represent a vital class of materials, with polyurethanes being a particularly versatile type, which are widely used in various industries. They are commonly synthesised from polyols and isocyanates, forming materials with diverse applications, including coatings, adhesives, foams, and elastomers. While bio-based polyols and glycols have been successfully introduced, replacing petrochemical isocyanates remains a significant challenge due to issues related to availability, cost, and scalability. The development of bio-based isocyanates is therefore of crucial importance if the sustainability of the materials is to be enhanced by reducing the reliance on petrochemical feedstocks and thereby reducing the environmental impact [1]. One strategy for optimising these materials is through chemical modification to tailor their properties, such as reactivity, solubility, and thermal stability [2].

The growing demand for sustainable materials has driven the development of bio-based isocyanates as environmentally friendly alternatives to petroleum-derived counterparts. In this study, a series of modified bio-based triisocyanates was obtained by selectively blocking one NCO group of a PDI-trimer using bio-methanol, ethanol and butan-1-ol as blocking agents. The resulting blocked isocyanates were characterized using Fourier-transform infrared spectroscopy (FTIR) and nuclear magnetic resonance (NMR) spectroscopy to confirm their chemical structure. High-performance liquid chromatography-mass spectrometry (HPLC-MS), MALDI-TOF and gel permeation chromatography (GPC) were also employed to analyse their molecular weight distribution, composition, and structural properties. Additionally, their thermal stability was evaluated through thermogravimetric analysis (TGA). The influence of the chosen blocking agents on the structural and thermal properties of the obtained isocyanates is discussed, providing insight into their potential applications in sustainable polymer synthesis.

The findings contribute to the ongoing efforts in creating bio-based materials with tailored properties, supporting the transition toward greener and more sustainable chemical production.

Acknowledgments
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The effect of a single methylene group in the spacer of liquid crystalline epoxy resin

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Keywords: LCER, mesophase, DSC, POM, thermal properties

The molecular design of liquid crystalline epoxy resins (LCERs) plays a crucial role in determining their mesophase stability and potential applications in advanced polymer networks. In this study, two LCERs with molecular spacers of 10 and 11 carbon atoms were synthesized to investigate the influence of a single methylene group on their phase behavior and structural characteristics.

The synthesized LCERs were structurally confirmed using proton nuclear magnetic resonance spectroscopy (^{1}H NMR). Their phase transitions and thermal properties were analyzed using differential scanning calorimetry (DSC), while the mesophase textures were examined by hot-stage polarized optical microscopy (hs-POM). The results demonstrated that both synthesized compounds exhibit thermotropic nematic liquid crystalline phase, confirming their potential as LC building blocks for functional polymeric materials.

A key finding of this study is that the length of the molecular spacer significantly influences the stability of the liquid crystalline phase. The LCER with the shorter, 10-carbon spacer exhibited a broader and more thermally stable mesophase range compared to its 11-carbon counterpart. These observations indicate that decreasing the spacer length enhances mesophase stability, which is a crucial consideration for tailoring the properties of LCER-based polymer networks.

The insights gained from this study contribute to a better understanding of the relationship between molecular architecture and phase stability in liquid crystalline epoxy resins. These findings provide a foundation for designing LCERs with optimized properties for use in advanced self-healing, reprocessable, and high-performance polymer networks. Future research will explore the incorporation of these LCERs into vitrimeric and crosslinked systems to assess their dynamic properties and potential applications in sustainable and smart polymer materials.

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Physicochemical characterisation and applications of biocatalyst based on chitosan hydrogels

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Keywords: chitosan, hydrogels, chymotrypsin, physicochemical characterisation

The immobilization of enzymes has numerous advantages that have allowed their successful use in industrial, pharmaceutical, chemical and biochemical processes. Immobilized enzymes are easily separated from the reaction mixture, can be reused, have high activity and are resistant to environmental changes. [1]. The properties of the immobilized enzymes are influenced by the properties of the support materials and of the enzyme itself. The chosen support must be chemically, physically and biologically stable during immobilization, as well as under reaction conditions, in order for the biocatalyst to exhibit excellent specific mechanical, chemical, biochemical and kinetic properties [2]. Biopolymers, such as chitosan or alginate, are among the many supports being studied for enzyme immobilization due to their unique properties (e.g. non-toxic, biodegradable and biocompatible, high affinity towards proteins, etc.) [3, 4].

The aim of the experimental study was to immobilize chymotrypsin on chitosan-based microspheres, namely pristine chitosan, glutaraldehyde-activated chitosan and chitosan and alginate microspheres. Chymotrypsin (EC 3.4.21.1) is an endopeptidase, with a molecular mass of 25 kDa, which hydrolyzes peptides containing tyrosine, tryptophan and phenylalanine residues [5]. The obtained microspheres were characterized by FT-IR spectroscopy, thermogravimetric (TG) analysis and scanning electron microscopy (SEM). The size and swelling capacity of the microspheres were also determined. To optimize the obtained biocatalyst, the influence of enzyme solution concentration on enzyme immobilization was investigated. The effect of pH and temperature on the activity of free and immobilized enzyme was studied. The experimental results showed that chymotrypsin was successfully immobilized on chitosan microspheres and the obtained chitosan microspheres are effective supports for the immobilization of chymotrypsin.

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Comparative kinetic study of the melt polymerization of isomeric dinitriles monomers by thermal analysis

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Keywords: diaminofumaronitrile, diaminomaleonitrile, melt polymerization, DSC, kinetic, mechanism

Nitrile compounds are abundant, stable, cheap, and readily available natural and chemical industrial sources. However, the effective conversion of nitrile monomers to functional polymers is limited due to their low reactivity, thus the development of efficient polymerizations based on them under very mild conditions is still a big challenge. In this context, dinitriles monomers represent an important subclass, where many of them, mainly of aromatic nature, are precursors of covalent triazine frameworks, possessing semiconductive properties, and being wide used in gas adsorption and separation as well as (photo)catalyst. The properties of this type of functional materials strongly depend on the type of monomers and the synthesis process, being the ionothermal polymerization one of the synthetic methods most used, which requires the presence of acid catalysts and high temperatures (> 400 ºC) [1]. However, the oligomers of hydrogen cyanide (HCN), such as the trimer aminomalononitrile and the two tretramers, diaminomaleonitrile (DAMN) and diaminofumaronitrile (DAFN) are less known, and their polymerizations, thought they have been scarcely studied, take place at lower temperatures and without the presence of initiators or catalysts. DAMN and DAFN are the *cis* and *trans* isomers, of 2,3-diamino-2-butenedinitrile, respectively; and they are of interest in research on the origin of life as well as astrobiology and, currently, in materials science. Herein, themoanalytical measurements have successfully described the bulk polymerization of DAFN in comparative discussion with its *Z* isomer; whose thermal polymerization in bulk, both in solid-state and melt, was previously studied through thermal analysis [2,3]. Simultaneous differential scanning calorimetry (DSC)-thermogravimetry (TG) and *in situ* mass spectrometry (MS) analyses reflected great similarities between them. Thus, two DSC series of nonisothermal experiments demonstrated that the DAFN polymerization is initiated at temperatures lower than the melting point, ~ 185 °C, when low heating rates (βs) are applied. On the contrary; higher βs results in a rapid polymerization reaction, which occurs entirely in the liquid phase. Both dynamic and isothermal DSC data were analysed using model-free linear iso-conversional methods to estimate kinetic parameters, such as activation energy, and a suitable kinetic model was proposed for these thermal polymerizations from the melt. A preliminary structural characterization by means of Fourier transform infrared (FTIR) spectroscopy was also completed. This study demonstrated the autocatalytic, highly efficient and straightforward character of this stimulated thermal polymerization of DAFN and, to the best of our knowledge, describes for the first time a systematic and extended kinetic analysis to gain mechanistic insights into this process. The latter was done through

the analyses of the gas products generated during these melt polymerizations, revealing that not only deamination and dehydrocyanation processes are two pertinent reactions involved in DAFN polymerization mechanism, but the thermal decomposition of the monomer itself could also affect the initiation.

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Bio-based diisocyanates - synthesis, characterization and application

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Keywords: bio-based diisocyanates, Curtius rearrangement, succinic acid, azelaic acid, sustainable production

Currently, polyurethanes (PUs) constitute an essential component of the plastics industry, with their versatility, durability and insulating properties, which render them indispensable in numerous applications. PUs are characterized by a segmented structure, comprising soft segments derived from polyols and hard segments primarily formed by isocyanates. Commercially available diisocyanates (e.g. MDI, pMDI, TDI, HDI, HMDI, IPDI) are predominantly of petrochemical origin and are synthesized via phosgenation of primary amines and their salts [1]. The primary drawbacks associated with petrochemical isocyanates include the high toxicity of phosgene, as well as their volatility and hazardous nature. Although significant progress has been made in the development of bio-based alternatives for polyols and chain extenders, commercially viable plant-derived diisocyanates remain scarce, and scientific literature on this topic is limited [2,3]. The objective of this study is to synthesize a fully bio-based diisocyanates from succinic acid (SA) and azelaic acid (AA) characterize their physicochemical properties, and assess its potential applications.

The synthesis of a linear aliphatic bio-based diisocyanate was performed using the Curtius rearrangement (CR). In the first step, succinic acid (SA)/azelaic acid (AA) was converted into dichloride via its reaction with thionyl chloride in the presence of DMF as a catalyst. In the second step, an acyl azide was obtained through the addition of sodium azide. Finally, the bio-based diisocyanate was formed by thermal decomposition of the resulting acyl azide. As a result, bio-based ethylene and octamethylene diisocyanates were successfully synthesized.

To determine and verify the chemical structure, the samples of bio based isocyanates were characterized using Fourier Transform Infrared Spectroscopy (FTIR) and Nuclear Magnetic Resonance Spectroscopy (^{1}H NMR, ^{13}C NMR). Thermal properties were further examined using Thermogravimetric Analysis (TGA). Furthermore, the NCO content was quantified by titration.

Obtained diisocyanates were examined for their usefulness in polymer synthesis. The successful synthesis of a fully bio-based diisocyanates from succinic and azelaic acid provides new insights into polyurethane chemistry and the market for its components. This path represents another step toward the development of fully sustainable polyurethanes.

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Thermal properties of bio-based thermoplastic polyurethanes subjected to multiple processing and recycling cycles

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Keywords: thermoplastic bio-polyurethanes, multiple processing cycles, mechanical recycling, sustainable development

Significant transformations are occurring in the economy, both nationally and globally, to reduce the harmful effects of industry on the environment. To support this transition, modern, environmentally friendly and sustainable technologies are being developed. With the increasing trend towards the production of plastics, green polyurethane materials made from plant-based components are gaining increasing attention. Particularly crucial are recyclable plastics that align with the principles of the circular economy [1]. Thermoplastics are the cornerstone of the plastics market due to their versatility in processing methods such as injection moulding, extrusion or casting, which enable high production efficiency. Among them, thermoplastic polyurethane (TPU), has gained widespread use in the automotive, footwear, electronics and medical industries [2] because of its desirable properties, such as transparency, elasticity, resistance to oil and grease, hydrolytic stability, microbe resistance, and low abrasion.

This study aimed to develop bio-based thermoplastic polyurethanes (bio-TPUs) and assess their recyclability over several consecutive cycles. Novel thermoplastic bio-poly(ether-urethane) materials, containing approximately 80% of bio-based content, were synthesized via a solvent-free, two step prepolymer method. The synthesis of base bio-material was carried out using bio-based monomers like: polyol poly(trimethylene glycol), bio-1,3-propanediol, and a diisocyanate mixture comprising hexamethylene diisocyanate (HDI) and a partially bio-based diisocyanate containing of 32% green carbon. Reference materials were ground and reprocessed in a closed mixer, undergoing four successive recycling cycles. This reprocessing method represented a form of mechanical recycling. The thermal properties of both reference and reprocessed materials were analysed after each cycle using thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), and thermomechanical properties by dynamic mechanical thermal analysis (DMTA).

A key finding of this study is that bio-based TPUs exhibit no significant degradation in properties after multiple processing cycles, providing new insights into the recyclability of thermoplastic polyurethanes.

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T22: Pyrolysis

Evaluation on gasification performance of waste tires based on chemical equilibrium analysis and ReaxFF-MD simulation

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Keywords: gasification, waste tires, styrene-butadiene rubber, chemical equilibrium analysis, ReaxFF-MD, DFT

The expansion of the automobile industry and transportation sector has led to a continuous and substantial growth in global automobile production. In 2019, the global vehicle production reached 95 million, which is expected to rise to 110 million units by 2025. The global production of waste tires (WT) has encountered a considerable challenge in terms of disposal and recycling due to their highly resistant nature to biological and chemical degradation. Gasification emerges as a promising option for the effective recycling of WT. The gasification of WT is searched mainly through experimental approach. Most investigation based on the chemical equilibrium analysis focus on the gasification of different biomass and coal in terms of temperature and feed concentration. DFT methods are extensively used in elucidating the microscopic reaction mechanisms involved in pyrolysis and combustion. The gasification mechanisms of WT at various atmosphere (weak oxygen, steam) are rarely reported in views of chemical equilibrium analysis along with ReaxFF -MD simulations and DFT. The gasification of WT was evaluated based on chemical equilibrium analysis in terms of reaction temperature (500 °C-1000 °C) and two atmospheres (oxygen: at equivalence ratio (ER) of 0.05-0.2; steam: at ER of 0.3-0.6;). Elevating temperature enhanced the formation of H_2 and CO in gasification of WT. Increasing oxygen concentration facilitated the production of CO, while impeded the generation of H_2, while increasing steam concentration promoted the synthesis of H_2 and CO. In addition, the temperature-dependent influence on the gasification degradation efficiency (DE) and the distribution of gaseous products from styrene-butadiene rubber (SBR) was determined at the molecular level based on reactive force field molecular dynamics (ReaxFF-MD) simulations and density functional theory (DFT) calculations. The optimal reaction paths for gaseous product generation were delineated. The optimal reaction path for generating H_2 was the reaction of 1,3-butadiene monomer with one H radical to produce 1,3-butadiene radical (FR6) and H_2 (ΔG=-111.55 kJ/mol). The best path for CO generation was the reaction of acetylene radical with oxygen radical (ΔG=-442.67 kJ/mol). The maximum degradation efficiencies in weak oxygen gasification and steam gasification of SBR were 67.03% and 68.46%, respectively. This study could provide basic data for the gasification of waste tires.

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Pyrolysis of waste rubber into sustainable biofuels using solar energy

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Keywords: pyrolysis, solar energy, waste rubber, bio-oil, bio-char yield, environment

The increasing worldwide demand for energy and the dwindling supply of fossil fuels have exacerbated the need for alternative energy sources. Waste rubber plays an important role in addressing present and future energy concerns, as well as meeting the growing need for sustainable energy sources. Besides, it addresses an environmental challenge when reused, and disposal decisions are avoided instead. Pyrolysis of discarded rubber presents a promising approach for generating sustainable energy. This study investigated the effect of temperature during the pyrolysis process on yield (syngas, bio-oil, biochar), physicochemical qualities, and energy production. This was accomplished using a solar-powered pyrolysis apparatus, and the feedstock was waste rubber with particle sizes ranging from 0.01 to 0.1 mm. Experimental and thermodynamic evaluations were carried out at temperatures ranges of 300 to 600°C, with heating rates of 10°C per minute. The results showed that increasing the pyrolysis temperature increased the bio-oil and syngas yields while decreasing the solid yield. The maximum biochar yield (32%) was achieved at 300°C. Furthermore, bio-oil yield reached 45% for particle sizes less than 0.01 mm, while syngas production reached 15% at 600°C. The produced bio-oil showed an average viscosity of 2.56 mPa·s and a density of around 1.07 g/cm³ under all circumstances. Chemical and physical parameters were determined using FTIR, GC-MS, FESEM, and EDX, which revealed the presence of CO, H_2, CH_4, and CO_2.

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Solar driven pyrolysis for the production of biofuels: an experimental study

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Keywords: pyrolysis, solar energy, biomass, syngas, biofuel, GHG, bio-oil

The pyrolysis of biomass employing solar energy for the production of biofuels is covered in detail in this study. Bioenergy has emerged as major short- and medium-term alternative to fossil fuels, presenting a substantial promise for decreasing greenhouse gas (GHG) emissions as the world's energy demand continues to rise fast and fossil fuel stocks continue to deplete. The most practical technique for converting biomass into biofuels is believed to be thermo-chemical conversion. Combustion, torrefaction, pyrolysis, hydrothermal liquefaction, and gasification are applicable methods used in this process. Three main products are typically produced by the pyrolysis in particular: bio-oil, biochar, and syngas. Under this investigation, solar cells were used to power the pyrolysis reactor, which pyrolysed biomass. Temperatures between 350 and 550 °C were used for the pyrolysis process, which was carried out under various operating conditions. Using the slow pyrolysis process, about 27% bio-oil and 43% biochar were produced in the products. Furthermore, the impact of several catalysts on the pyrolysis process was examined. Results revealed that the use of a catalyst improved the yield and quality of the bio-oil. A temperature of 550 °C was found to be the optimum operating condition, yielding the largest amount of bio-oil.

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Oxidative pyrolysis of Refuse-Derived Fuel (RDF): a kinetic study

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In Colombia, the daily generation of solid waste is estimated at approximately 33,000 tons, of which about 90% ends up in landfills and open-air dumps. The rest is dumped in bodies of water, soils, and ecosystems, which generates serious environmental pollution. This inadequate waste management contributes to 15% of greenhouse gas emissions in the country. In this context, the Colombian government has committed to reducing its total emissions by more than 40% by 2050, in line with global sustainability goals. To address this problem, various initiatives have been developed aimed at waste recovery [1,2]. In the La Miel landfill, located in Ibagué, Colombia, an innovative technology has been implemented that allows waste to be transformed into a combustible material suitable for thermal processes such as pyrolysis [3]. This work aims to evaluate the oxidative pyrolysis of a combustible waste derived from waste (CDR) in order to determine its viability as a sustainable energy source. The obtained material was characterized by calorific value analysis (HHV), elemental analysis, and immediate analysis. It was then subjected to an oxidative pyrolysis process using a TA Instruments thermogravimetric analyzer (TGA). The results showed that the material has an adequate calorific value and a significant content of fixed carbon and volatile matter, which guarantees good performance in thermal processes. Furthermore, despite the inherent heterogeneity of the material, low levels of sulphur and nitrogen were identified. This implies that emissions of polluting gases such as NO_x and SO_x would be minimal during its combustion. In conclusion, this study demonstrates the potential of the derived combustible residue as a viable alternative to reduce dependence on fossil fuels and minimize the environmental impacts associated with inadequate waste management. The larger-scale implementation of similar technologies could significantly contribute to national and international climate change mitigation and environmental sustainability goals.

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Advancing biochar-based catalysis for hydrogen production: a systematic review on activation strategies and recent developments

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Keywords: biochar, catalyst, activation, hydrogen production

The global transition toward sustainable energy sources has intensified the interest in hydrogen (H_2) production as a clean and renewable alternative fuel. Biochar, a carbon-rich material derived from various thermochemical conversion approaches using different types of biomass, has recently emerged as a promising catalyst for hydrogen production. Its distinctive structure, high surface area, porosity, and functionalizable surface chemistry make it an attractive candidate for hydrogen production applications. The activation and functional modifications of biochar catalyst could further improve the hydrogen yield and quality, thus enhancing its catalytic activity. Despite its growing potential, the application of biochar as catalyst or catalyst supports for biomass upgrading and hydrogen production has not been systematically reviewed. This review presents a comprehensive review of the biochar production technologies, activation and modification strategies and the role of biochar as a catalyst for hydrogen production. It explores the recent advancements in utilising biochar as a sustainable and cost-effective catalyst for clean energy applications. The insights presented aim to advance the research in biochar-based catalysis, contributing to the development of efficient and environmentally friendly hydrogen production technologies.

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T24: Thermal conductivity

Thermal properties and lattice disorder effects in ZnMnTe crystals using photopyroelectric calorimetry

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Keywords: crystal growth, ZnMnTe crystals, photopyroelectric calorimetry, thermal conductivity, lattice disorder

Broadband solid solutions of II-VI compounds are of significant interest both for theoretical exploration and for practical applications in modern optoelectronics. However, their physical properties remain largely unexplored due to the complexity of their preparation technology. Despite this, II-VI mixed crystals remain important for contemporary electronics, optics, and spintronics, as they offer the possibility of manipulating material properties such as energy gap and lattice constant. Current research focuses on a variety of applications, including solar cells[1], photodetectors for different wavelengths[2],], and light-emitting structures[]

Zinc manganese telluride, a type II-VI semiconductor with a tunable bandgap, is attracting considerable interest due to its diverse applications, including nuclear radiation detectors and industrial process monitoring. This study investigated the thermal properties of $Zn_{1-x}Mn_xTe$ ternary semiconductors obtained by the vertical Bridgman-Stockbarger growth method over a Te content range from 0 to 0.5. The composition of the samples was determined using the energy dispersive analysis (EDS) technique. X-ray diffraction (XRD) was used to characterize the crystalline structure of the material.

Thermal studies were also carried out using the photopyroelectric calorimetry (PPE) technique [4]. The thermal diffusivity and effusivity values were extracted from the experiment, allowing the calculation of the specimens' thermal conductivity using the Adachi model.

The results show that the thermal diffusivity and conductivity of the studied materials decrease as the Mn content in $Zn_{1-x}Mn_xTe$ increases. Based on these measurements, it can be concluded that the incorporation of Mn into ZnTe crystals has a significant impact on their thermal properties These results provide valuable information on the thermal properties of $Zn_{1-x}Mn_xTe$ compounds and contribute to a better understanding of their behavior in different fields of application.

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Study of thermal proprieties and surface state of CdS_xTe_{1-x} and $CdMg_xTe_{1-x}$ using photothermal methods

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Keywords: thermal characterisation, CdTe based semiconductor crystals, piezoelectric photothermal spectroscopy, photopyroelectric technique (PPE)

Cadmium telluride-based materials are one of the most promising semiconductor materials being considered to create convenient X-ray and γ-ray detectors. For these materials, it is possible to change electronic properties, lattice parameters, and band gap energies by adjusting the composition of the mixed crystals. The change of band gap energy gives the desired optical properties and emission in the spectrum's entire visible and UV range.

The crystal investigated in this work is the cadmium sulfide telluride (CdS_xTe_{1-x}) with sulfide content of $0 \leq x \leq 0.1$, and the cadmium magnesium telluride ($Cd_{0.95}Mg_{0.05}Te$). The samples were grown from the melt using the vertical Bridgman Stockbarger method. The crystals are characterized using two photothermal methods, each associated with a different nature of generating the photothermal signal. The piezoelectric photothermal spectroscopy (PPS) enables measurements in the front and reverse configurations and applies a piezoelectric detector to measure the photothermal signal. It is sensitive to the surface preparation of the sample [1] and enables the determination of the optical properties of the materials. The photopyroelectric technique (PPA) is a contact method that directly measures heat oscillations [2] and allows for the determination of thermal properties (thermal diffusivity and effusivity).

The spectra from the piezoelectric photothermal spectroscopy shows a strong influence of surface preparation on the characteristics of the spectra can be seen. It varies with the modulation frequency, which allows us to estimate the thickness of the defective surface layer and develop an appropriate surface treatment method. Cd1-xSxTe is a new material, and we present one of the first results of the obtained thermal parameters.

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Thermophysical properties evaluation on polymers and phase change materials: a systematic study

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Keywords: thermophysical properties, specific heat capacity, thermal diffusivity, thermal conductivity, polymers, phase change materials

The accurate determination of thermophysical properties - such as thermal conductivity, thermal diffusivity, specific heat capacity and density - is crucial for understanding heat transfer phenomena in materials. The accuracy in the determination of these properties is often underestimated and issues in repeatability of the results are common in the scientific community. Thermophysical properties are strongly dependent on temperature, hence their evaluation is affected by testing condition and thermal inertia effects. Moreover, thermophysical properties are often indirectly determined through the measurement of other correlated physical quantities, with the disadvantage of the error propagation that has to be taken into account. Many techniques have been developed for the determination of specific heat capacity, thermal diffusivity and thermal conductivity, however, it is common to obtain results without a clear convergence between the different procedures, in particular if testing parameters are selected without a deep knowledge of the consequences of a wrong selection.

This study explores various experimental techniques to determine the thermophysical properties form 0 °C to 90 °C of widely studied thermoplastic polymers, as high-density polyethylene (HDPE) and expanded polystyrene (EPS), in order to compare, if available, the obtained results with those published in literature. This work has been then extended to the characterization of the thermophysical properties both of the solid and liquid phase of phase change materials (PCMs). These materials are increasingly used in various energy applications and, in particular, as suitable materials to be integrated into thermal energy storage (TES) systems. The investigated PCMs are eicosane, an oligomer selected as pure substance, and a fatty acid mixture which can better represent a commercial type of PCM.

Differential Scanning Calorimetry (DSC) was used to determine specific heat capacity following ASTM E1269-11 standard, relating the heat flux of the samples with that obtained from a sapphire reference, whose specific heat capacity is known as function of temperature, and the results obtained at different scanning rates from 10 to 0.1 °C/min were compared. A recent alternative to the conventional scanning calorimetry technique was also exploited, a method which overlays ramped temperature with a time series of stochastic temperature pulses of different durations (TOPEM) [1]. Various heating rates and pulse heights were probed, relating the accuracy and the reliability of the obtained results.

Thermal diffusivity was measured through a Laser Flash Analyzer (LFA)[2] following ASTM E1461-13 and independently with Hot Disk measurement following ISO 22007. Thermal conductivity was an output of hot disk measurement or indirectly determined as product of diffusivity (from LFA), specific heat capacity (from DSC) and bulk density of the

material. A third technique to measure thermal conductivity is the heat flow meter (HFM) method following ISO 8301[3], in which a temperature gradient is imposed to the material. This method could be used only for insulating materials, as in the case of EPS.

We propose a critical discussion relatively to the different strategies and parameters to determine these thermophysical properties, underlying their advantages and disadvantages, with the aim to highlight the methodological difficulties and to stress the importance of the great accuracy needed for thermophysical properties determination.

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Fast determination of the thermal conductivity of insulating materials

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Keywords: thermal conductivity, insulating materials, refractory materials, rapid measurement, experimental methodology

Nowadays, there is a rapid and dynamic development of renewable energy sources (RES), particularly photovoltaics, which has been growing at an average annual rate of 24%, with an exceptional increase of 36% in 2023. These trends are expected to bring about dramatic changes in the energy sector. One potential solution to this evolving situation is the implementation of high-temperature heat storage systems. This research is dedicated to exploring this concept, focusing on the study and development of suitable materials for high-temperature energy technologies. The investigation primarily addresses two key areas: insulating materials for high-temperature applications and thermal storage materials.

From the perspective of thermal insulation materials, the thermal conductivity coefficient (k) is the decisive parameter. This parameter, in general terms, depends on temperature, density, chemical composition, material structure, pressure, and humidity. It is defined as the amount of heat passing through a unit area of an isothermal surface per unit of time under a unit temperature gradient within the material. The thermal conductivity coefficient is essentially specific to each type of material. A crucial characteristic of this parameter is its temperature dependence. In high-temperature applications, the significant increase in thermal conductivity with rising temperature is a critical consideration. For high-temperature insulation materials, thermal conductivity plays a crucial role in determining performance. Defined as the rate of heat transfer through a unit area under a unit temperature gradient, thermal conductivity is highly material-specific. In high-temperature applications, its tendency to increase with rising temperatures is a critical consideration, as higher thermal conductivity can lead to undesirable heat dissipation.

For certain widely used materials, such as steel and glass, numerous empirical models exist for estimating thermal conductivity. These models incorporate the chemical composition of the material and often allow for the calculation of conductivity as a function of temperature. However, for heterogeneous materials, such simplifications are not feasible. In such cases, precise experimental measurements are required to obtain reliable thermal conductivity values. This is particularly crucial for materials with either very high or very low conductivity, as accurately characterizing these properties necessitates meticulous determination of the relevant physical parameters.

This research aimed to identify materials suitable for high-temperature applications in the energy sector. The focus was directed toward two key areas: insulation materials designed for high-temperature environments and materials intended for thermal storage. The study presents an innovative methodology for rapidly determining the thermal conductivity coef-

ficient and evaluates its application across a series of material samples. The findings indicate that, for optimal retention of thermal energy (sensible heat and enthalpy), the most effective approach is to use insulation materials with both a low thermal conductivity coefficient and a low thermal diffusivity coefficient. This combination minimizes heat transfer between the storage system and its surroundings, ensuring that the thermal potential of the reservoir remains at a functional level for extended periods. Additionally, the study highlights potential material modifications that could enhance both the insulating and mechanical properties of these materials.

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Performance of solar distillation systems with reflectors: a comprehensive review

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Keywords: desalination, solar stills, reflectors, solar energy, water scarcity

Solar distillation is a promising and environmentally friendly method for producing potable water, especially in arid and remote regions. Enhancing the efficiency of solar stills is crucial to meet growing water demands. This paper comprehensively reviews solar distillation systems integrated with reflectors, focusing on their performance improvements. By concentrating sunlight, reflectors enhance the thermal input to the distillers, thus increasing water evaporation rates and overall system productivity. Various reflector designs, materials, and configurations are examined to understand their impact on distillation efficiency. The review also highlights recent innovations and experimental results, comparing the performance of systems with and without reflectors under different climatic conditions. So, this paper provides insights into optimizing solar distillation systems for better water output and sustainability by summarizing key findings and identifying research gaps.

T25: Thermal hazards, lifetime prediction

Thermooxidative stability of polymers employed in the conservation of plastic artefacts

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Keywords: thermooxidation, thermooxidative stability, residual stability, polymers, DSC

In many applications of everyday life it is necessary to find the most suitable materials in terms of their thermooxidative stability. Moreover, it is often necessary to examine the effect of different types of ageing and/or their combinations on the stability of materials. It is obvious that assessing the thermooxidative stability of materials under different conditions is a time-consuming process and it is often impractical to use common procedures in the initial evaluation of the stability. Thus, there is a demand for fast screening methods for evaluating the stability of many materials under the influence of various environmnetal factors.

In this work we have applied a fast procedure for quantifying the effects of elevated temperature in the presence of air on the stability of various polymers that could be applicable for the lifetime estimation of the artefacts made of plastics. Samples of polyethylene, polypropylene and polystyrene aged at 80 °C in the presence of air were used as model materials and were studied using non-isothermal DSC measurements. For the treatment of the experimental results, a method for the evaluation of the kinetic parameters describing the temperature dependence of the induction periods of thermal oxidation based on non-Arrhenian temperature function, was employed[1]. From the kinetic parameters the lengths of induction periods and subsequently the residual stabilities[2] of the samples have been calculated.

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Effects of $Ca(H_2PO_4)_2$ and $(NaPO_3)_6$ on the suppression of wheat flour dust explosions

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Keywords: food dust explosion, flame retardant, explosion sensitivity, thermogravimetric analysis, thermal stability

Wheat flour, rice and corn, among other grains, pose a risk of food dust explosions during production and processing. This study investigates the inhibitory effects of two food-grade flame retardants, monocalcium phosphate ($Ca(H_2PO_4)_2$) and sodium hexametaphosphate ($(NaPO_3)_6$), on wheat flour dust explosions. A 20-L explosion sphere was used to measure the minimum explosion concentration (*MEC*), maximum explosion pressure (P_{max}), and maximum rate of pressure rise ($(dP/dt)_{max}$). The minimum ignition energy (MIE) was also tested to assess electrostatic sensitivity. The results indicate that adding 10% flame retardant did not effectively reduce the MEC, but a 20% concentration increased the MEC, thereby reducing explosion sensitivity. Among the two, $(NaPO_3)_6$ illustrated superior explosion suppression compared to $Ca(H_2PO_4)_2$, with an 8:2 ratio reducing P_{max} from 7.9 barG to 7.3 barG and lowering $(dP/dt)_{max}$ by 34%. Additionally, within the dust concentration range of 750–1,000 g/m³, $(NaPO_3)_6$ exhibited better explosion suppression, while $Ca(H_2PO_4)_2$ had a more considerable effect at concentrations above 1,250 g/m³. Regarding MIE results, both flame retardants notably increased the minimum ignition energy of wheat flour from 660 mJ to over 1,000 mJ, thereby reducing explosion sensitivity. A simultaneous thermal analyser (STA) was used to conduct thermogravimetric analysis, and the apparent activation energy was calculated using advanced thermal analysis software (AKTS). Both flame retardants enhanced the thermal stability of wheat flour, with $Ca(H_2PO_4)_2$ performing the best, increasing the apparent activation energy by approximately 50 kJ/mol. Overall, the 8:2 ratio is the most effective and is recommended for reducing explosion risks in food processing. Future studies can explore its long-term stability, suitability for different powders, and effectiveness at high concentrations to enhance food safety standards.

Acknowledgments
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Research on the thermal stability of painted layers on wooden substrates

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Keywords: alkyd paints, natural ageing, environmental factors action, exposure time increasing, TGA, DSC

Wood, especially fir, is being used more and more in building homes and other structures because it offers a good balance between cost and quality. To protect wood, it needs to be treated with coatings like paints and varnishes. These coatings are made of dyes, organic and mineral pigments mixed into a binder, which, once dried, form a long-lasting, flexible, and shiny protective layer [1]. This study aimed to understand how these coatings change over time and how much they degrade after being exposed to the environment for 6, 12, and 18 months. The thermal stability of the coatings was tested using thermogravimetric analysis and differential scanning calorimetry. Three types of alkyd resin-based coatings were studied: SLT (a rosewood-colored varnish with Teflon), ECM (a mahogany-colored water-based coating with acrylic resins), and LYP (a clear urea-alkyd yacht varnish).Samples were applied in one or two layers and exposed to four different climates with varying rainfall, sunlight, and temperature changes, as well as in a controlled lab setting with stable temperature and humidity. Over time, exposure to these conditions caused changes in the coatings due to polymer breakdown, cross-linking, and oxidation. These chemical changes affected both the mechanical properties and the stability of the coatings [2, 3].

Only small changes in thermal stability were noted for samples exposed in the PN area, which has a temperate continental climate with short, cool summers, long autumns, and mild winters. These changes occurred regardless of exposure time or the number of coating layers applied to the fir wood boards. The most significant thermal changes were observed in samples exposed in the IS area (figure 1), which has a predominantly continental climate with hot, dry summers and cold winters, often experiencing blizzards due to northern and northeastern air masses. Similar effects were seen in the CT area, where the presence of the Black Sea and the Danube leads to high humidity and temperature regulation, resulting in average temperatures 11.2°C higher than in other regions. For the water-based ecolasure (ECM), which contains alkyd and acrylic components, exposure to high temperatures had a noticeable impact. Additionally, regarding elasticity, the protective alkyd varnish with Teflon (SLT) showed reduced flexibility after 6 months of environmental exposure compared to samples kept in controlled lab conditions for the same period.

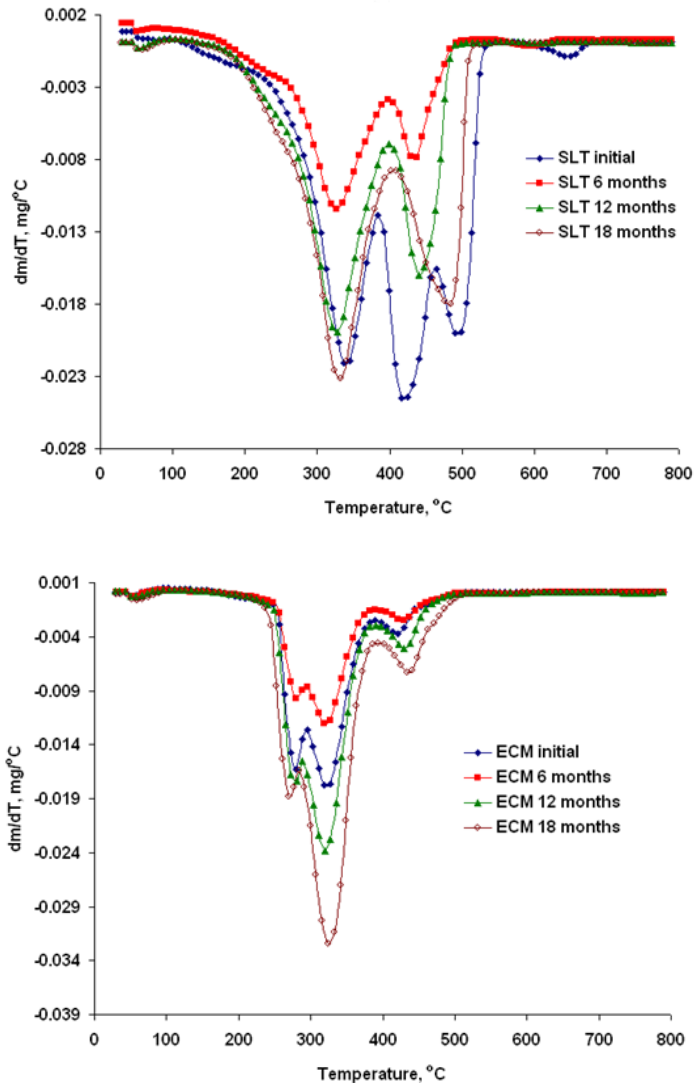

Figure 1. DTG analysis of SLT and ECM samples with two coats exposed in the IS region

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Impact of different cyclic/linear electrolyte compositions on the thermal runaway of lithium-ion batteries

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Keywords: electrolyte, structural compositions, charge-discharge cycling test, thermal runaway, decomposed gases

The electrolyte plays a crucial role in determining the performance and safety of lithium-ion batteries (LIBs). This study investigates how different structural compositions of electrolytes impact battery behavior by fabricating full cells with varying electrolyte formulations. The batteries underwent a charge-discharge cycling test to evaluate their electrochemical performance. In addition, their thermal runaway characteristics were examined under adiabatic high-temperature conditions using an Accelerating Rate Calorimeter (ARC) and a vent aizing package (VSP2). The decomposed gases generated during LIB decomposition at high temperatures were identified using gas chromatography-mass spectrometry (GC-MS) to further analyze safety risks. Key thermal runaway parameters, such as the onset temperature (T_{onset}), maximum temperature (T_{max}), maximum pressure (P_{max}), temperature rise rate (dT/dt), and pressure rise rate (dP/dt), along with the gas composition, were analyzed. Finally, the correlation between electrolyte structural composition, battery performance, and safety is discussed based on the experimental results, providing insights for future LIB thermal runaway prevention.

Acknowledgments
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T26: Thermochemistry

Migration and occurrence mechanism of trace metallic elements and compounds in an enhanced thermal treatment of irradiated graphite: insights from chemical equilibrium analysis

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Keywords: spent nuclear graphite, metallic nuclide, thermal treatment, chlorides and bromides, chemical equilibrium analysis, response surface methodology

Spent nuclear graphite is a key radioactive waste material generated during the decommissioning of high-temperature gas-cooled reactors. Compared with incineration, chemical treatment and other treatment methods, the thermal treatment has the virtues of simplicity, sustainability, and low carbon emissions. Thermal treatment is a promising technology for decontaminating spent NG by separating radioactive isotopes and impurities, which can recover precious metallic nuclides and also provide the possibility of recycling graphite. With the growing global demand for rare isotopes, the recovery of main metallic radionuclides and some uranium and transuranium elements would provide valuable energy for special fields. In current work, the migration and transformation mechanism of the trace metallic and compounds in nuclear graphite in enhanced thermal treatment were estimated based on chemical equilibrium analysis in terms of temperature and additives (chlorides and bromides).NH_4Br was determined to be the optimal brominating agent between 633 K to 1023 K, since NH_4Br could effectively convert metallic nuclides (Ca, Fe, Co, Ni, Cs, Sr, Eu, U, Pu) into gaseous bromides with the molar ratio of NH_4Br to metallic nuclides of 100:1. The decontamination temperatures of most metallic radionuclides declined with increasing NH_4Br addition in the range of 1:1-200:1. The main products for Ca, Fe, Ni, Cs, Sr, Eu and U were $CaBr_2$ (g), $FeBr_2$ (g), $NiBr_2$ (g), NiBr (g), CsBr (g), $SrBr_2$ (g), $EuBr_2$ (g) and UBr_4 (g). The decontamination efficiency of 99 % for metallic nuclides 99% was achieved with minimal NH_4Br or $MgCl_2$ addition, outperforming conventional chlorinating agents (NaCl, $CaCl_2$). The chlorination effects of NaCl and $CaCl_2$ for metallic nuclides were very weak. However, $MgCl_2$ emerged a strong chlorination action. The complete volatilization temperatures for Fe, Co, Ni and Cs were lower than 1053 K with a 3.89% (mass fraction) $MgCl_2$ addition. Key factors that influence decontamination efficiency, including temperature range (573 K-1673 K), additives (NH_4Br, $MgCl_2$, NaCl, $CaCl_2$) and their molar ratio (1:1-200:1), were systematically investigated via response surface methodology (RSM). The temperature had the most significant impact on the decontamination efficiency, followed by molar ratio and type of additives. The

optimal parameters regarding maximum gaseous metallic compound yields stemmed by Ca, Fe, Ni, Cs, Sr, Eu and U were 1123 K, NH_4Br and the molar ratio of 100:1, respectively, while the optimization trials under RSM-guided conditions regarding maximum gaseous metallic compound yields derived from Co and Pu were 1512 K, $MgCl_2$ and the molar ratio of 171:1, respectively. This work could attribute to an enhanced thermal treatment and basic guidance for decontamination of the radioactive metallic elements and compounds in the irradiated graphite.

Acknowledgments
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T27: Fire dynamics (or others for fire safety)

Thermal analysis of flame-retarded polylactic acid composites during composting

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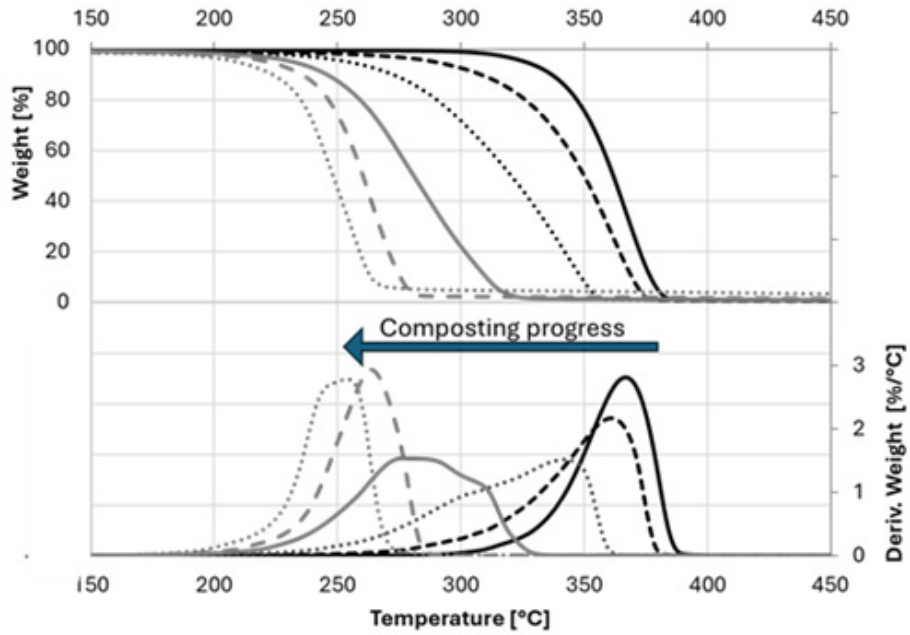
Keywords: polylactic acid, composting, flame retardant, additives

Polylactic acid (PLA), a bio-based polyester derived from renewable sources, has gained attention due to its biodegradability and industrial compostability; however, the incorporation of commonly used additives such as flame retardants and cellulose fibres can alter its degradation characteristics.

In this study, the thermal behaviour of flame-retarded PLA composites was investigated to understand the influence of various additives on their degradation and compostability. PLA composite systems were prepared using Ingeo™ Biopolymer 3052D grade polymer and ammonium polyphosphate (Exolit® AP 422, AP 462), melamine polyphosphate (Budit® 341), cellulose fibres (Arbocel UFC 100, B600), a chain extender (Joncryl ADR-4468), and bentonite (CLOISITE® 116) additives, respectively. The composites were fabricated as hot-pressed sheets and CO_2-assisted batch-foamed structures, then subjected to controlled composting conditions according to ISO 20200:2004. Differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), and Fourier-transform infrared spectroscopy (FTIR), were employed to monitor the degradation process at different intervals.

The results revealed that processing techniques, sample morphology, and additive composition influenced compostability, with variations observed in the decomposition rates of different formulations. The findings provide insights into optimizing PLA-based flame-retardant materials for enhanced sustainability without compromising thermal stability and degradation performance.



TGA and DTG curves of a PLA sample during the composting procedure

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Development of alginate-based flame retardant systems for poly(lactic acid)

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Keywords: polymers, flame retardancy, alginate, phytic acid, PLA

Nowadays, the environmental and ecological damage caused by fossil-based plastic waste is receiving increasing attention. Pollution can be significantly reduced by replacing fossil-based plastics with biopolymers such as poly(lactic acid) (PLA). PLA is a versatile, biodegradable, and compostable biopolymer that is emerging as a leading alternative to non-biodegradable and non-renewable synthetic plastics. However, due to PLA's flammability and melt-dripping properties, safety regulations in certain technical applications require it to undergo flame-retardant treatment.

The most recent advances in research and development focus on incorporating bio-based functional additives into polymeric materials at an increasing ratio. Alginate (Alg), a readily available bio-sourced compound extracted from brown seaweed, is a suitable starting material for such purposes. Among other applications, complexes of alginic acid with metal ions have been successfully used as carbonizing agents in intumescent flame-retardant systems [1].

During our work, we used phytic-acid (PA) – a bio-based compound with high phosphorus content – to chemically modify sodium alginate and develop an effective, bio-based flame-retardant system, which can be used to reduce or replace the amount of less environmentally friendly flame retardants in PLA. By numerous experiments, the pH value, the ratio of the reagents and the method of the precipitation of the alginate hydrogel with calcium-ions – and thus the particle size – were optimized. Then, the precipitation reaction was scaled up in order to ensure a more economic production process.

The newly synthesized additive – containing alginate and Ca-phytate in a 1:2 weight ratio – was comprehensively analyzed using thermal analysis and spectroscopic methods, while the morphology and structure of the additive were evaluated using scanning electron microscopy coupled with energy dispersive X-ray spectroscopy.The flame-retardant effect of the selected additive embedded in a PLA matrix was evauated using standard testing methods such as UL 94 flammability test, Limiting Oxygen Index (LOI), and Cone Calorimetry (CC).

The PLA composite containing 7.5 wt% ammonium-polyphosphate (APP) and 7.5 wt% of the new additive reached V-2 classification according to the UL 94 test. By using 7.5 wt% of the modified alginate instead of sodium alginate beside 7.5 wt% APP in PLA matrix, the LOI value has increased by 4.5%. During the CC tests of the PLA composites, 15 wt% of the newly produced additive in the PLA reduced the total smoke emission during the combustion by about 60% compared to the composite that contained 15 wt% of APP.

The investigation of the effects of the change in the specific surface area with the further physical modification of the alginate complexes – with methods such as electrospinning, lyophilization and foaming – on the flame rertardant performance is currently in progress.

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Extinguishing performance of a water mist with primary linear alcohols additives: a physical analysis

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Keywords: water mist, alcohol additives, pool fire, engine compartment

Vehicle fires are a major issue for critical road transportation such as ambulances, buses, fire-fighter trucks, or military vehicles. The main sources of fires in vehicles are electrical or mechanical failures. The engine compartment is particularly vulnerable due to the presence of combustible materials and fluids, as well as numerous hot spots that can easily reach temperatures of several hundred degrees Celsius. New regulations for noise and pollution levels lead to an overall higher temperature inside the engine compartment [1]. Nowadays, the protection of engine compartments in military vehicles is performed using total flooding gas systems like the HFC-277ea. The gas is clean and safe but is environmentally persistent and has a substantial global warming potential. In line with the present environmental efforts towards carbon neutrality and the Kigali Amendment to the Montreal Protocol, alternatives to the current fire protection system must be found. One such alternative can be the water mist system. The water mist system for fire suppression has demonstrated its potential and effectiveness to extinguish many fire classes. Water mist is clean and safe for human beings and the environment. However, it remains to be seen if the water mist system is suitable for the protection of an engine compartment. The fire protection of such a confined space presents additional constraints in terms of water volume and pressure, as retrofitting a large pump would not be feasible. The performance of the water mist system must be found elsewhere.

The characteristics of the sprayed solution itself can be modified using additives. An additive for water mist is understood as any species that is added to the spray. Additives are usually required: to tackle certain classes of fire, such as cooking oils and fats or gas, to decrease the droplet size, or to disturb the chain reaction of combustion. A review of the available literature unveils a gap in the research for additives acting in a physical way [2]. Besides surfactants, which are commonly used in the formulation of fire-fighting foams, a new category of additives has been identified in solvents and alcohols. Paradoxically, these flammable species have been found to be effective additives for water mists, notably through the work of Koshiba et al. [3] and more recently Xu et al. [4]. A trend within primary linear alcohols has been identified by Koshiba et al. but was not investigated further. In the present study, the use and fire extinguishing mechanisms of primary linear alcohols as additives for water mist on an n-heptane pool fire will be investigated from methanol to 1-heptanol at volume fractions from 0.6% to 20%. After a physical analysis is conducted, a model for the prediction of extinguishing time is developed based on alcohol characteristics. Finally, the performance of alcohol additives is compared with hydrocarbon surfactants.

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T28: Thermal imaging

Hot-stage microscopic analysis of strzegom granites in the context of their chemical composition and thermal properties

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Keywords: granites, hot-stage microscopy, mineralogical characterization, sintering behavior, functional optimization

During granite crushing, large amounts of fine fractions with a grain size of less than 2 mm are created. They are most often mined due to the significant share of the dust fraction, and less frequently used during production, e.g. as a backfill material.

Therefore, this work aims to determine their thermal properties, based on Hot-Stage microscopic (HSM) studies of six samples of fine granite fractions from southwestern Poland, from the Strzegom-Sobótka massif. These studies confirmed that the alkali content significantly reduces all characteristic temperatures, as well as viscosity at temperatures above 1000ºC. On their basis, raw materials that can be used as a flux in ceramic masses with a dark body, as well as a raw material for reducing and improving the sinterability of clay masses, were selected.

The most favourable parameters were obtained for samples with the highest sodium feldspar content from Chwałków (sample 1232) and Gola Świdnicka (1234).

In addition, the melt viscosity curves were determined by the experimental method (HSM) and from the chemical composition by the Bottinga-Weill method. In the temperature range of 1200º-1400ºC, a correlation of results can be seen, but the viscosity determined by the first method is about 2 dPas higher.

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