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CATCAR33

17-18 of October 2024, Timişoara – Romania

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PLENARY LECTURER

PL1
PROCESSING MATERIALS WITH ELECTRIC FIELDS

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PL2
ISOCONVERSIONAL KINETIC ANALYSIS OF THERMAL DECOMPOSITION OF BIODEGRADABLE POLYMER BLENDS

Stefano VECCHIO CIPRIOTI[1], Jacopo TIRILLÒ[2], Fabrizio SARASINI[2]
Tibor DUBAJ[3]
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INVITED LECTURE

IL 1
THERMAL CHARACTERIZATION OF COMPOSITE MATERIALS FOR 3D PRINTING

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IL 2
INSIGHTS INTO NANOCOLLOIDS FOR HEAT TRANSFER APPLICATIONS

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IL 3
THERMAL EVOLUTION OF POLYPHASIC CERAMIC FLUE GAS SORBENTS

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ORAL PRESENTATION

OP1
RECENT CONTRIBUTIONS TO PREFORMULATION OF HORMONAL COMPOUNDS USED IN THERAPY

Ionuț LEDEȚI[1], Amalia RIDICHIE[1,2*], Cosmina BENGESCU[2], Laura SBÂRCEA[1], Cornelia MUNTEAN[2], Gerlinde RUSU[2], Răzvan BERTICI[1,3], Florentin CRĂINEANU[3], Francisc PETER[2], Adriana LEDEȚI[1]

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OP2
UNRAVELING THE CATALYTIC BEHAVIOR OF VARIABLE-VALENCE MIXED METAL OXIDES CATALYSTS BY *IN SITU* ELECTRICAL CONDUCTIVITY MEASUREMENTS

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OP 3
HISTORY OF THERMAL ANALYSIS & THERMAL ANALYSIS OF HISTORY

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OP 4
GENERALIZED CONVERSION FUNCTIONS IN HETEROGENEOUS KINETICS

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OP 5
PREPARATION AND STUDY OF LOW-COST ENVIRONMENTAL POLLUTION ADSORBENTS FROM SPENT TYRE

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OP 6
THE STUDY OF HETEROGENEOUS PROCESSES OF PREPREG COMPOSITE MATERIALS BY THERMAL AND KINETIC ANALYSIS

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OP7
RATIONAL DESIGN OF REACTIVE NATURAL DEEP EUTECTIC SOLVENTS TO ENHANCE ESTERIFICATION ACTIVITY AND THERMAL STABILITY OF LIPASES.

Alina R. BUZATU[1,2], Anamaria TODEA[1,*] Raluca O. POP[2], Diana M. DREAVĂ[1], Cristina PAUL[1], Ioan BÎTCAN[1], Marilena MOTOC[2], Francisc PETER [1], Carmen G. BOERIU[1,*]

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POSTER SECTION

Theory & Methods, Kinetics & Structural Changes.

P1

THERMOLYSIS OF FOUR SARTANS: KINETIC ANALYSIS BASED ON THERMOGRAVIMETRIC DATA

Adriana LEDEŢI[1*], Amalia RIDICHIE[1], BIANCA BAUL[2], CARMEN TOMOROGA[1], GABRIELA VLASE[3], TITUS VLASE[3], Ionuţ LEDEŢI[1,2]

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P2

SOLID-STATE STABILITY AND KINETIC ANALYSIS OF FLUOROMETHOLONE

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P3

THERMAL STABILITY AND KINETIC STUDY OF IRBESARTAN

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Calorimetry of Polymers, Bio(macro)molecules, Life science and Organic Functional Systems with medical applications

P4

THE INFLUENCE OF CO-SOLVENT ON CYCLODEXTRIN COMPLEXATION: STUDY ON CARVEDILOL

Ema NIŢU[1], Ioana MITROFAN[1], Luciana BULIGA[1], Amalia RIDICHIE[1], Adriana LEDEȚI[1], Cornelia MUNTEAN[2], Gerlinde RUSU[2], Gabriela VLASE[3] Denisa IVAN[1], Carmen TOMOROGA[1] Ionuţ LEDEȚI[1], Laura SBÂRCEA[1]

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P5

PRELIMINARY STUDIES OF SOME NEW POSSIBLE PHARMACEUTICAL FORMULATIONS WITH DRUGS FROM THE ANTICOAGULANT CLASS

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P6

PREPARATION AND CHARACTERISATION OF INCLUSION COMPLEX OF LEVONORGESTREL WITH SULFOBUTYLETHER-BETA-CYCLODEXTRIN

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P7

EVALUATION OF INTERACTIONS BETWEEN POLYMER-GELATIN HYDROGELS AND PROPYPHENAZONE

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STUDY OF POLYMER-BASED JELLIES FOR ANTIPYRETIC AND ANALGESIC DRUG

Ionela-Amalia BRADU[1,2], Mihaela BUDIUL[1], Gabriela VLASE[1,2], Mădălina GRĂDINARU[1,2], Alexandru PAHOMI[1], Titus VLASE[1,2]

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COMPARISON OF THE BIOLOGICAL ACTIVITY OF THE ARILS, SEEDS AND MIXTURE OF TAXUS BACCATA

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PHYSICOCHEMICAL AND ANTIOXIDANT CHARACTERISATION OF A FOOD SUPPLEMENT BASED ON GINGER (*Zingiber officinale),* IN VITRO EVALUATION

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INSIGHT INTO THE PHYSICOCHEMICAL AND THERMAL BEHAVIOR OF NEW MICROCARRIERS BASED ON ROMANIAN WILD-GROWING *Inonotus obliquus*

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FUNCTIONAL MATERIALS, CERAMICS, METALS & ALLOYS, CEMENTS AND ENGINEERING MATERIALS & COMPOSITES

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EXPERIMENTAL RESEARCH ON THERMAL-ELECTRICAL BEHAVIOUR OF LANTHANUM MANGANITE COMPOUNDS

Paula SFIRLOAGA[1], Gabriela VLASE[2], Titus VLASE[2], Ionel BALCU[1], Corina MACARIE[1], Doru BUZATU[1]

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Beatrice VLAD-OROS[1], Daniela DASCĂLU[1], Iarina ION[1], Alexandru PAHOMI[1,2], Ionela-Amalia BRADU[2,3], Gabriela VLASE[2,3], Titus VLASE[2,3]

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EXPLORING THE POTENTIAL OF BLACK LIQUOR AS A REINFORCING AGENT FOR MODERN ADOBE BRICK COMPOSITES

Dorinel OKOLIŠAN[1], Titus VLASE[1,2], Ionela-Amalia BRADU[1,2], Gabriela VLASE[1,2], Aurelian GRUIN[3,4], Cornelia BAERĂ[3,5], Vlad STANCIU[6]

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HERITAGE AND ARCHAEOLOGICAL STUDY

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THE STUDY OF RED PIGMENTS IN POWDER FORM AND MIXED WITH BINDERS USING PHYSICAL AND CHEMICAL INVESTIGATIONS

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A COMPARATIVE STUDY BETWEEN BLUE PIGMENTS FROM ORIGINAL PAINTING LAYERS AND CONTEMPORARY REPLICAS

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THERMAL AND HYPHENATED TECHNICS IN THE STUDY OF PIGMENTS USED IN PAINTINGS

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STATISTICAL ANALYSIS OF HERITAGE OBJECTS DATA ACQUIRED BY PHYSICO-CHEMICAL TECHNIQUES

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SOIL PHOSPHATE ANALYSIS OF ARCHAEOLOGICAL SOIL FROM ARAD COUNTY

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THE USE OF MULTIPLE TECHNIQUES IN THE INVESTIGATION OF SOME FRAGMENTS OF DACIAN CERAMICS, DISCOVERED NEAR THE DACIAN FORTRESS OF ALUN-PIATRA ROȘIE (HUNEDOARA COUNTY)

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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 HYPHENATED TECHNIQUES

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BEYOND THE MOUNTAINS: ANALYSIS OF BRONZE AGE POTTERY SAMPLES FROM THE VÂNĂTORI-NEAMȚ - *VALEA REA* FORTIFICATION (VÂNĂTORI-NEAMȚ, NEAMȚ COUNTY, ROMANIA) USING MULTIPLE ANALITIC TECHNIQUES

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PLENARY LECTURES

PROCESSING MATERIALS WITH ELECTRIC FIELDS

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Electromagnetic fields, as alternative to conventional heating, for materials processing is an interesting topic that has raised the interest of the scientific community in recent times. Moreover, processes induced by electrical fields present specific features that are not achieved in conventional heating processes. Thus, electromagnetic fields could promote far from equilibrium processes not achievable by conventional procedures. Lately, it has been reported that zirconia can be sintered within seconds just by applying small DC fields. This procedure has been named Flash Sintering (FS) and it has been extended to a the sintering of a significant number of ceramic materials, including ionic and electronic conductors, insulators, ferroelectric, multiferroic, piezoelectric, structural, non-oxide ceramics, metastable compounds, etc. Moreover, ceramics processed using FS have interesting microstructures and nonequilibrium defects that yield, in some cases, peculiar unexpected properties. Experimental conditions such as the use of DC or AC fields or different current controlled modes can be used to tailor the microstructrure and properties of the resulting materials.

Recently, it has been shown the possibility of inducing concomitant chemical reactions and sintering during one single experiment in few seconds. This procedure has been used for the preparation of different types of ceramics: ferroelectric, multiferroic, piezoelectric, high entropy oxides, solid state ionic conductors, complex nitrides, chalcogenides, etc.

This new field has also raised the interest of industry as it might be used in electrification of industrial production processes in continuous mode reducing the energy consumption and the carbon footprint of ceramic production.

ISOCONVERSIONAL KINETIC ANALYSIS OF THERMAL DECOMPOSITION OF BIODEGRADABLE POLYMER BLENDS

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In recent years, many studies have been devoted to the kinetic analysis of thermal decomposition processes of a wide range of materials using both very old and more recent methods. The ICTAC kinetic Project' group led by Sergey Vyazovkin has provided recommendations via valuable reviews [1-3] on how to process experimental thermal analysis data and monitor the most important operating conditions, aiming to discourage authors from using unreliable approaches. However, some aspects of this "classical" approach are still controversial and some clarifications are needed.

In this study, starting from a general overview of the pros and cons of using some isoconversional methods, we aimed to shed new light on the kinetic descriptions of pyrolysis occurring in neat polymers (poly(lactic acid), poly-(3-hydroxybutyrate-co-3-hydroxyvalerate) and poly-(butylene-adipate-co-terephthalate) denoted as PLA, PHBV and PBAT, respectively), and in two of their binary and ternary blends [4]. To carry out a suitable kinetic analysis, a mathematical deconvolution (according to the Fraser-Suzuki peak function) was performed on integral curves and the deconvoluted curves were analyzed separately by the isoconversional method. This isoconversional analysis of deconvoluted temperature dependence of conversion curves allows calculating some parameters for the assessment of the potentially accelerating or inhibiting effect on thermal decomposition, for example, by the half-time ($t_{0.5}$) decomposition.

Finally, the effect of blending on the thermal stability of the tested blends for each constituent was evaluated. In particular, the stability of PHBV in binary and ternary blends was improved compared to the neat polymer.

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INVITED SPEAKER

THERMAL CHARACTERIZATION OF COMPOSITE MATERIALS FOR 3D PRINTING

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Polymer was the defining material of the twentieth century whilst, both for the considerable increase in articles published in literature and for the growth of applications over the last fifteen years the defining material platform of the twenty-first century could very well be the hybrid material. The design of an hybrid material is related with the combination of two or more components in a single material to give new and previously unattainable combinations of useful properties [1].

Among the different techniques available, thermal analysis offers, in addition to high accuracy in the measurement, smartness of execution, allowing to obtain with a very limited quantity of material precious information regarding the property–structure correlation, essential not only in the production process, but overall, in the design one. Thus, techniques such as differential scanning calorimetry (DSC), differential thermal analysis (DTA), dynamic mechanical analysis (DMA) and thermogravimetric analysis (TGA) can be used in the design, preparation and characterization of these materials.

Furthermore, since the public pressure about the problems derived from the environmental issues increasingly pushes the research areas, of both industrial and academic sectors, to design material architectures with more and more foundations and reinforcements derived from renewable sources. In these efforts, researchers make extensive and profound use of thermal analysis to this transition from fossil feedstock to renewable ones, and in the development on new manufacturing processes such as those of additive manufacturing (AM).

AM is increasingly in industry with a worldwide market, for AM products and services, estimated to grow to over $5 billion by 2020 [2]. AM is accepted not for prototyping only but for functional parts too [3], and the filament based technology referred as the Fused Deposition Modelling (FDM) is one the most widely used. Thermal analysis can be used to study the behavior of polymer melts, and not only, during FDM processing to rationalize its effect on printing quality.

The research was partially funded by the European Union (NextGeneration EU) and MUR-PNRR project Sicilian MicronanoTech Research And Innovation Center – SAMOTHRACE (CUP E63C22000900006), Spoke 1, WP 1.6.2 and partially funded by the MUR under the grant scheme PRIN with the project TARGET “addiTive mAnufactuRing for liGhtwEight joinTs” (grant number 2020E3XL47_003, CUP E63C20011220001).

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INSIGHTS INTO NANOCOLLOIDS FOR HEAT TRANSFER APPLICATIONS

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Abstract. Heat transfer enhancement is a relentless concern in the last years due to the continuous necessity of dropping down the overall energy feeding and equipment miniaturization, as well [1]. Therefore, the development of new heat transfer fluids is a must of these years' industrial progress. Essentially, the idea of developing innovative fluids started from the low thermal conductivity of basic heat transfer fluids and their conceivable upgrading through the insertion of high conductive solid nanoparticles, leading to the so-called "nanoparticle enhanced fluids" or "nanofluids", named lately as "nanocolloids". There is tremendous work on nanocolloids, while most of these fluids are based on water and ethylene glycol. This paper will go into less studied nanocolloids having ionic liquids (IL) and polyethylene glycol (PEG) as potential substitutes for conventional heat transfer fluids. The main advantages of ILs and PEGs is their stability at higher temperatures, being able to perform above 100 °C.

Among all the possible thermal energy applications [2], solar energy harvesting highlights as the candidate in which ILs and especially nanoparticle enhanced ionic liquids perfectly fit. Certainly, this kind of fluids possess the general qualities required in these systems, principally low vapor pressure to ensure that the fluid remains in the liquid state during operation and high thermal stability to resist the temperatures reached in a solar collector. Common heat transfer fluids, such as water or glycols, would vaporize at these temperatures leading to structural and heat transfer issues in the solar installations. Moreover, nanocolloids with IL have proofed to achieve higher augmentations in global heat transfer performance than nanocolloids based on water, as confirmed by Prasad et al. [3]. If it discusses the possible applications of PEGs, Minea [4] reviewed the properties of several PCMs with nanoparticles dispersed in polyethylene glycols with different molar mass. The main objective of the review was to discuss the influence of nanoparticles addition on the thermophysical properties of the polyethylene glycol. Also, the study revealed a moderate increase in viscosity while thermal conductivity and specific heat increase. Furthermore, PEG 400 with different nanoparticles were studied over the years in terms of thermophysical properties and benefits and drawbacks were discussed by Chereches et al. [5].

As a general conclusion of the experimental studies on using nanocolloids with ionic liquids and PEG as future heat transfer fluids the advantages are clear in terms of thermal stability, lack of sedimentation and thermal conductivity enhancement, while the main issue remains the increase in viscosity and the high price of these chemicals.

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THERMAL EVOLUTION OF POLYPHASIC CERAMIC FLUE GAS SORBENTS

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A mixed metal oxide system was investigated as a gas sorbent for the desulphurisation at high temperatures within integrated gasification combined cycle process. The sorbent was based on Zn, Ti, Al in various rations, because; Zn phases may support sorption, Ti phases may support chemical stability and Al phases may support mechanical durability. The preparing route comprised sol-gel synthesis with complexing agent to control the hydrolysis rate. The formation and decomposition of related chelates was quite complex, thus the insight in the process advancement, has been enabled by the structural (NMR, FTIR, XRD) and thermal analyses (DTA-TGA).

The precursor alkoxides react completely with the complexing agent forming chelates. One day old gels are already quite hydrolysed; the hydrolysis is faster with zinc nitrate hydrate phase present, as the water needed for hydrolysis if supplied. Samples with minor titania are composed of layered double hydroxide while in samples with greater amount of titania nitrates crystallise. The stability ranges of the observed solid-solutions were confirmed through the structure refinement. Partial phase-separation at occurred at mild thermal treatment, which affected the high temperature phase development. An intermediate Zn-based phase was found to be responsible for the facilitated early zincite crystallisation.

The materials were investigated for specific application of sulphurous gasses removal from the hot flue gas application. We sulphured the thermally treated samples thereby simulating the hot flue gas processing, we monitored the thermal and structural properties of sulphurous gasses-saturated samples in order to observe and clarify different mechanisms of phase formation as a function of the starting composition, subsequently we regenerated the sorbents in TGA at air atmosphere. Zinc sulphide spinels and zinc sulphide dominate in the samples. Conversion, stability and durability behaviour were evaluated. Finally, we were able to confirm thermal treatment at 500 °C and composition of $Zn_7Al_2Ti_3O_{14}$ fit the best for a hot flue gas desulphurisation application.

Acknowledgement: This work was funded by the CSF under the project UIP-2019-04-2367.

ORAL PRESENTATION

OP 1
RECENT CONTRIBUTIONS TO PREFORMULATION OF HORMONAL COMPOUNDS USED IN THERAPY

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Hormone therapy represents a medical approach that use hormones as active pharmaceutical ingredients in the treatment of different conditions, including hormonal therapy for cancer, hormone replacement therapy for menopause, androgen replacement therapy, contraception and sex reassignment therapy [1,2].

This presentation deals with our recent contributions to the instrumental investigations of hormonal compounds used in different pathologies, by thermal and spectroscopic tools, mainly in the development of new solid dosage forms with improved stability and bioavailability.

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OP2
Unraveling the catalytic behavior of variable-valence mixed metal oxides catalysts by *in situ* electrical conductivity measurements

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The semiconductive and redox properties of variable-valence mixed metal oxides play a key role in catalytic reactions involving a heterogeneous redox mechanism, such as selective and total oxidation [1, 2], the *in situ* electrical conductivity measurement being a highly sensitive and useful technique to study them [3]. Indeed, as a heterogeneous redox mechanism implies the reduction and re-oxidation of the oxide during the catalytic cycle, useful information can be obtained by following the evolution of the electrical conductivity of the solid catalyst as a function of the nature of the gas phase in contact with it, including the reaction mixture, at a temperature within the reaction temperature range. For example, in the presence of a reducing gas, such as hydrogen, carbon oxide or a hydrocarbon, which consumes lattice oxygen species, the electrical conductivity increases or decreases for an *n*-type or a *p*-type oxide, respectively, compared to that under an oxidizing gas flow, such as air or oxygen. The observed effects give relevant information about the redox properties of the oxide helping unravel its catalytic behavior.

We employed this technique to investigate several variable-valence metal oxides used as catalysts in various processes, such as oxydehydrogenation and partial oxidation of light alkanes [4-6], total oxidation of different pollutants like methane, ethylene, soot [7-9] preferential oxidation of CO [9] and autothermal reforming of ethanol [10]. The results obtained allowed us to establish correlations between the semiconductive and redox properties of the examined oxides and their catalytic performance in the considered process, and to unravel the origin of their catalytic behavior, which may stimulate new ways of catalyst design. In this presentation, the most relevant of these results will be covered.

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OP 3
HISTORY OF THERMAL ANALYSIS & THERMAL ANALYSIS OF HISTORY

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Thermal analysis at UVT started in the year 1992 using a MOM derivatograph. Later, the equipment continuously evolved, reaching the purchase of a complete line in 2005 within the "Center for Thermal Analysis in Environmental Problems" and then in 2022 a high-performance line was purchased at ICAM-UVT.

The articles published in ISI journals that used thermal analysis studies followed in a way certain trends specific to the research area, i.e. initially studies of the compensation effect and studies of the support effect were carried out with the help of kinetic methods, then followed by thermal stability studies of complex combinations, oils, environmental studies, flame retardant compounds, polymer compounds, substances with biological activity, food additives, drug substances, nanomaterials and nanocomposites with predetermined properties. Throughout this period, the kinetic studies continued on all categories of samples analyzed and were continuously improved, culminating with the NPK method modified and perfected by Vlase T. Vlase G. and Doca N. In the last period, studies on samples of interest were approached archaeological, namely: pipes, mortars, ceramics, crucibles and paintings. Also of interest is the field of studies in the field of forensics, which is constantly developing.

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OP 4
Generalized conversion functions in heterogeneous kinetics

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Heterogeneous processes are regularly thermally-stimulated phenomena, when at least one condensed phase (usually a solid phase) participates to the overall process, generating their complexity. Thus, it is straightforward to acknowledge the unfolding of a heterogeneous process with single or multiple steps, including overlapping chemical reactions and physical processes (diffusion, nucleation & growth, etc.). Kinetic models are relevant to describe heterogeneous kinetic processes; a number of kinetic models and their mathematical expressions have been reported in the literature, many of these based on idealistic conditions in terms of geometrical constrain and driving forces. Alternatively, the semi-empirical Sestak-Berggren (SB) conversion function [1], which was proposed as a general equation, encompasses a large variety of equations corresponding to different kinetic models. Despite the fact that the SB equation does not provide any physical meaning, it is extremely useful for kinetic analysis as it offers a good fit to experimental data even when they do not follow the ideal conditions assumed for the conventional kinetic models [2]. Although the logarithmic part within the SB kinetic model is important (as in the case of historical kinetic models), it brings some impediments while playing the role of accommodation function at when $\alpha \to 0_+$ or $\alpha \to 1_-$. And last but not least, maybe the most important limitation is the fact that its conversion function cannot be analytically integrated to provide an exact solution; thus, it cannot be directly applied in kinetic integral methods.

In this study we aimed for a better understanding of the Sestak-Berggren (SB) generalized conversion function and proposed some solutions for certain specific cases [3], while the mathematical limits for the values of the kinetic exponents *m*, *n*, *p* of the SB model and their validity were also explored [3]. Moreover, we have approximated the SB conversion function with a new one (and also its consequent integral), which has the same behaviour and very important, the same extreme points of extreme (*i.e.* the maximum) [4]. Furthermore, an alternative for a superior conversion function – not related to the SB function – is also proposed.

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OP 5
PREPARATION AND STUDY OF LOW-COST ENVIRONMENTAL POLLUTION ADSORBENTS FROM SPENT TYRE

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Solid carbon residue, commonly known as carbon black, is a carbon-rich byproduct generated during the pyrolysis of rubber materials. Classified as a potential human carcinogen, short-term exposure to elevated levels of carbon black can cause discomfort and mechanical irritation in the upper respiratory tract. Addressing the environmental challenges posed by industrial waste, including carbon black, is essential for sustainable waste management solutions. One promising approach to enhance the utility of carbonaceous materials is activation, a process that modifies their surface properties through partial oxidation. This method utilizes agents such as steam, carbon dioxide, and alkali metal hydroxides or carbonates to create activated carbon with enhanced adsorption capabilities, offering potential for applications in pollution control and other environmental technologies.

This study aims to develop and characterize adsorbent materials derived from solid industrial waste, specifically from the pyrolysis residue of tires. A series of carbon-based adsorbents were produced using various physical, chemical, and thermal treatments to modify the waste materials and improve their adsorption properties. Activation was conducted in a horizontal reactor, with water vapor serving as the activation agent, alongside pre-treatments involving KOH, H_3PO_4, and HNO_3. The resulting adsorbents were characterized through gas adsorption measurements, IR spectroscopy, and thermal analysis, demonstrating enhanced properties for potential environmental applications.

The obtained results indicate the possibility of obtaining carbonaceous adsorbents with economic potential from solid waste generated during tire pyrolysis. This study highlights the feasibility of obtaining and characterizing adsorbent materials from solid industrial waste. The utilization of such materials not only offers a sustainable solution for waste management but also presents an opportunity to address environmental concerns and promote cleaner industrial practices.

OP 6
THE STUDY OF HETEROGENEOUS PROCESSES OF PREPREG COMPOSITE MATERIALS BY THERMAL AND KINETIC ANALYSIS

Didina-Ramona-Casandra CÂRSTEA[1,2], Jordi FARJAS[2], Daniel SANCHEZ-RODRIGUEZ[2], Sihem ZAIDI[2], Ahmed Mohamed SALEH ABD ELFATAH[2], Andrei ROTARU[3,4], Josep COSTA[2]

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Thick carbon-fibre-reinforced polymer (CFRP) laminates are of practical interest for manufacturing pressure vessels for hydrogen storage, pressure pipes, for the aerospace industry, or to strengthen structural elements. However, can lead to thermal gradients forming within a specimen.

A recurring problem when curing thick specimen carbon-fibre-reinforced polymers is the formation of thermal gradients, due to the combination of a high exothermal curing reaction together with the low thermal conductivity of epoxy resins. Thermal gradients can lead to heterogeneous properties, overcuring and, in some cases, matrix degradation. To address this problem, we have developed a general-purpose analytical solution that allows one to predict the maximum temperature difference within a specimen when the curing reaction takes place under isothermal conditions. The analytical solution is based on a heat diffusion model that takes convection heat losses into account; it is specifically tailored to deal with standard conditions in the manufacture of composites and can be applied to different resins and prepregs. Besides, the model also provides the critical thickness required to prevent a thermal runaway. The model is validated against numerical simulations and experimental data from the curing process of a CFRP with VTC401 epoxy component prepreg ("pre-impregnated" fibres with a partially cured polymer matrix). In addition, it allows one to determine the conditions for when a thermal runaway will occur. The model was validated after the analytical predictions were compared with the numerical and experimental results.

O7
RATIONAL DESIGN OF REACTIVE NATURAL DEEP EUTECTIC SOLVENTS TO ENHANCE ESTERIFICATION ACTIVITY AND THERMAL STABILITY OF LIPASES.

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Over the past decade, deep eutectic solvents (DESs) have gained considerable atention as a sustainable, green option for extraction and reaction media in biorefineries and various chemical and biotechnological applications. Particularly, reactions catalysed by enzymes are carried out in deep eutectic solvents as these solvents help to maintain high substrate solubility while improving both enzyme stability and efficiency. With molecular weights ranging from 1 to 50, natural deep eutectic solvents (NADES) are not only used as solvents for extracting bioactive compounds, but also as substrates and catalysts for reactions. This multifunctional approach with reactive NADESs (R-NADESs) opens the potential for improved biocatalytic and chemocatalytic processes with reduced downstream processing and low waste production [1,2].
This study reports on the beneficial effect of R-NADESs on the esterification activity and thermal stability of free and immobilised lipases in the synthesis of polyol- and carbohydrate-based biosurfactants. We prepared and characterised 18 binary and ternary R-NADES systems with ChCl as HBA and carbohydrate polyols, mono-, di- and oligosaccharides, urea (U), N-methylurea (MU) and water as HBD in different combinations and molar ratios. The composition of the mixtures, the molar ratio, the thermal properties, i.e. decomposition temperature (T_{dec}), water loss, melting temperature (T_m), glass transition (T_g) and viscosity were measured and the relationships between the different parameters were analysed and discussed. A large number of lipases, both native and immobilised lipases showed high stability and remarkable catalytic performance in RNADES solvents.

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POSTER SECTION

Theory & Methods, Kinetics & Structural Changes.

P1

THERMOLYSIS OF FOUR SARTANS: KINETIC ANALYSIS BASED ON THERMOGRAVIMETRIC DATA

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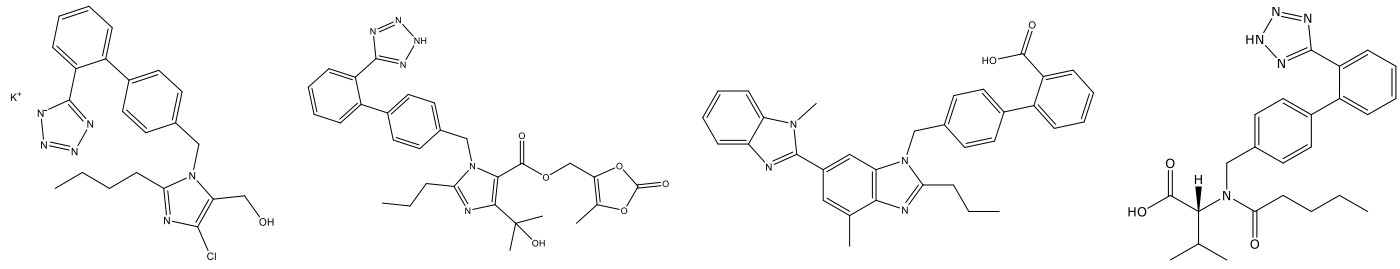
Angiotensin II receptor antagonists (sartans) are tetrazole derivatives used in the treatment of high blood pressure, being also indicated for the treatment of heart failure (NYHA class II-IV) in adults with left ventricular systolic dysfunction (ejection fraction = 40%) to reduce hospitalizations and death from cardiovascular causes [1,2]. After oral administration, the active substances are quickly absorbed, but their bioavailability is low, due to the first hepatic passage. To increase their bioavailability (from 4.5% to 28.6% in the case of olmesartan), esterified forms of the drugs have been developed, for example olmesartan is available as a prodrug in the form of olmesartan medoxomil, which is rapidly transformed in vivo in pharmacologically active olmesartan, also losartan is conditioned as a potassium salt, called losartan potassium.

The aim of this study was to evaluate the thermal stability and degradation kinetics for a series of sartans, namely telmisartan, valsartan, olmesartan medoxomil, and losartan potassium, to gather information regarding the thermal stability of the principal compounds used in therapy from this class. The kinetic methods used were the preliminary ASTM E698 method, respectively the isoconversional Flynn-Wall-Ozawa (FWO) and Friedman (FR) methods. Also, to obtain the kinetic triplet and for a better understanding of the mechanism underlying the degradation process the modified non-parametric (NPK) kinetic method was applied. The chemical structures of these sartans are shown in Figure 1.



Losartan potassium	Olmesartan medoxomil	Telmisartan	Valsartan

Figure 1. Chemical structure of the selected sartans

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P2
SOLID-STATE STABILITY AND KINETIC ANALYSIS OF FLUOROMETHOLONE

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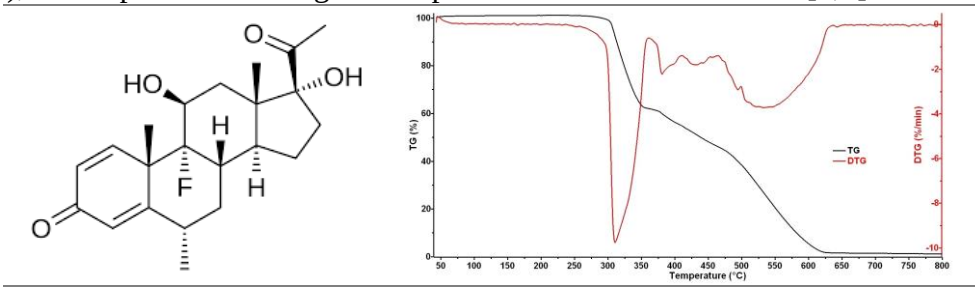
Fluorometholone (chemical structure presented in Figure 1a) is a commonly prescribed molecule for the treatment of the symptoms of dry eye in non-Sjogren and Sjogren's patients. It is a fluorinated corticosteroid, presenting outstanding advantages over the other compounds from this class, such as high pharmacological potency, a lower incidence in causing cataract or glaucoma, as well as a rapid corneal metabolism to minimize the systemic exposure after topical application. To diminish the dry eye sensation, fluorometholone increases the expression of mucin-1, mucin-4, mucin-16, and mucin-19, genes crucial for ocular hydration, lubrication and barrier function. It is available as an ophthalmic suspension, due to its extremely low aqueous solubility (approximately 0.009 mg/mL), which poses a challenge in the pharmaceutical formulations [1,2].



a **b**

Figure 1. (**a**) Chemical structure of fluorometholone, (**b**) TG and DTG curves of fluorometholone at β=10 °C/min

The purpose of this study is to evaluate the solid-state stability of fluorometholone by using the following instrumental techniques: ATR-FTIR spectroscopy and thermal investigations (TG/DTG and DSC) at five different heating rates β = 2, 4, 6, 8 and 10 °C/min (in Figure 1b are represented the TG and DTG curves registered at β=10 °C/min). To perform the kinetic analysis one preliminary kinetic method was used (ASTM E698) and three isoconversional methods, namely: Kissinger–Akahira–Sunose, Flynn-Wall-Ozawa and Friedman.

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P3
THERMAL STABILITY AND KINETIC STUDY OF IRBESARTAN

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Irbesartan is an orally active angiotensin II type 1 receptor antagonist, also known as an angiotensin receptor blocker (ARB). It has an imidazolinone ring, where a carbonyl group functions as a hydrogen bond acceptor instead of the hydroxymethyl group in losartan. Irbesartan was patented in 1990 and approved for medical use in 1997. It is available on the pharmaceutical market under the name Avapro [1]. Its pharmacological profile sets it apart from other drugs in the same class due to its high bioavailability and extended duration of action. It is particularly recommended for patients with renal insufficiency and has demonstrated significant efficacy in treating left ventricular hypertrophy and congestive heart failure, regardless of the stage of renal disease. Irbesartan is also indicated for managing hypertension and renal insufficiency in patients with type 2 diabetes (T2D) and hypertension [2] [3].

This study aims to examine Irbesartan's thermal stability based on its molecular structure, with the goal of synthesizing new materials for the controlled release of the active ingredient. The stability of the compound was evaluated at temperatures ranging from 25 to 400°C, with a heating rate of 5, 7, 10, 12, 15°C/min, in an atmospheric environment with synthetic air. The analysis was conducted using a Mettler TOLEDO TG/DSC3+ thermobalance in an open aluminum crucible. Kinetic analysis followed the ICTAC 2000 protocol, employing the Friedman, Ozawa-Flynn-Wall, Kissinger-Akahira-Sunose isoconversional, and modified nonparametric kinetic methods.

In order to support our study, we also used FTIR-U-ATR spectroscopy to analyze the compounds obtained by burning the active substance at different heating rates to determine the mechanism of its decomposition. FTIR-U-ATR spectroscopy data was collected using a Perkin Elmer SPECTRUM 100 device and employing the Universal Attenuated Total Reflectance (U-ATR) technique. Data collection was performed after 8 consecutive recordings at a resolution of 4 cm^{-1} on the spectral range 4000 – 650 cm^{-1} .

The study aimed to determine the kinetic triplet without approximations, while also identifying and separating parallel or successive reactions that occur during the decomposition of the active substance.

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Calorimetry of Polymers, Bio(macro)molecules, Life science and Organic Functional Systems with medical applications

P4

THE INFLUENCE OF CO-SOLVENT ON CYCLODEXTRIN COMPLEXATION: STUDY ON CARVEDILOL

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Carvedilol (CARV) is a representative of antihypertensive drugs, one of the most effective nonselective alpha-1 and beta blockers, commonly used in the current therapy of various cardiac pathologies such as mild to severe congestive heart failure, cardiac arrhythmias, myocardial infarction and angina pectoris. It also possesses antioxidant activity [1,2]. CARV belongs to the BCS class II, exhibiting high lipophilicity and poor solubility in water and gastrointestinal fluids that lead to low absorption and poor bioavailability, limiting its clinical potential [3]. In order to improve low solubility of drug substances several approaches can be employed, including micronization, cyclodextrin complexation, cocrystals formation, solid dispersions, surfactant system [4]. For enhancing CARV solubility, inclusion complexation of drug with randomly methylated β-cyclodextrin (RM-β-CD) was used.

In this study the effect of solvent systems on the inclusion complexation process of CARV was investigated. CARV/RM-β-CD inclusion complexes (ICs) were prepared using the kneading method in 1:1 molar ratio, employing water (IC1) and a mixture of water:ethanol absolute (1:1, m/m) (IC2), respectively, as solvent systems. The ICs were characterized in solid state using thermal analysis, attenuated total reflectance Fourier transform infrared (ATR-FTIR), powder X-ray diffractometry (PXRD) and also in solution by means of saturation solubility studies.

The results obtained from shake-flask method revealed an improvement in CARV solubility for both IC1 and IC2, with higher value for IC1. The PXRD investigation indicated an amorphization process in both ICs difractograms, supporting the ICs formation when using the both solvent systems. A greater reduction in intensity of CARV characteristic peaks was noticed in the case of IC1, in agreement with the results of solubility studies. For CARV/RM-β-CD ICs, the use of water when the kneaded method is employed leads to more intense host-guest interaction as compare to water:ethanol absolute solvent system.

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P5
PRELIMINARY STUDIES OF SOME NEW POSSIBLE PHARMACEUTICAL FORMULATIONS WITH DRUGS FROM THE ANTICOAGULANT CLASS

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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.

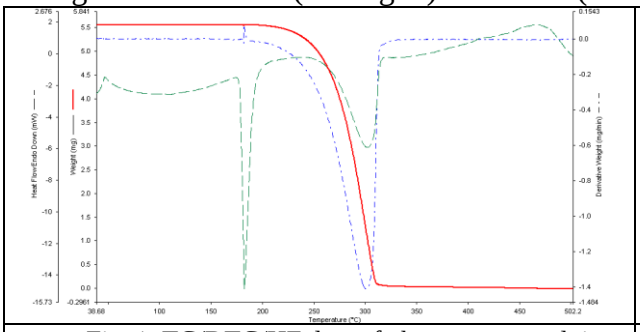

Fig. 1. TG/DTG/HF data of phenprocumonului

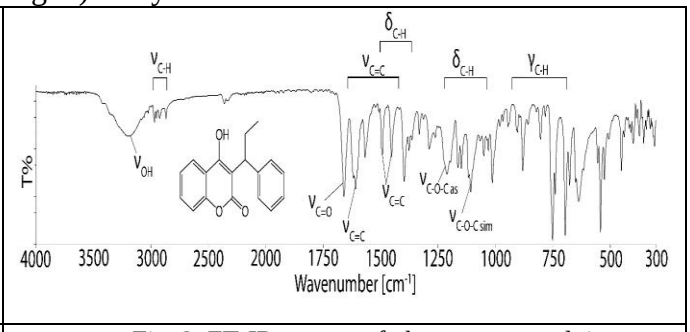

Fig. 2. FT-IR spectra of phenprocumonului

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P6
PREPARATION AND CHARACTERISATION OF INCLUSION COMPLEX OF LEVONORGESTREL WITH SULFOBUTYLETHER-BETA-CYCLODEXTRIN

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Levonorgestrel (chemical structure presented in **Figure 1**) is a derivative of progesterone, being included in the second generation of progestins [1]. It is used as a contraceptive, possessing a double mechanism of action, namely: the inhibition of ovulation and the thickening of the cervical mucus. Even if it is used in various oral dosage formulations (dragées, tablets, coated tablets and orodispersible tablets), in some cases the side effects, such as vomiting and nausea, prevented its use [2,3]. This inconvenience can be overcomed by dermal administration of the active pharmaceutical ingredient. Since patches present a low compliance from the patients, another dermal route is represented by microneedles [3]. In order to use levonorgestrel for this type of pharmaceutical formulation, is it necessary to increase its water solubility.

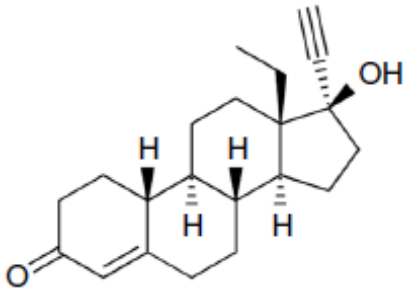

Figure 1. Chemical structure of levonorgestrel

The purpose of this study is to increase the solubility of levonorgestrel by forming an inclusion complex with a cyclodextrin, namely Sulfobutylether-beta-cyclodextrin sodium salt (DS~6.5). The obtained inclusion complex was subjected to phase solubility studies, Job's method and Benesi–Hildebrand method. Also, to confirm the formation of the complex several instrumental methods were approached: FTIR analysis, thermal analysis (TG/DTG, DTA) and PXRD analysis.

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P7
EVALUATION OF INTERACTIONS BETWEEN POLYMER-GELATIN HYDROGELS AND PROPYPHENAZONE

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Gelatine presents good biodegradability, non- toxicity with the human body and has a low cost. Due to its poor mechanical properties it can not be used in applications as a structural biomaterial, but presents valuable biopolymer properties for tissue engineering and drug delivery systems. Thus the reinforcement of gelatin materials becomes a challenge for the researchers and by using it in combinations with biopolymers that can give a stable 3-D microstructure by cross-linking we can obtain novel composites with enhanced properties [1].

This composites can be used for drug delivery systems and this research tried to incorporate a pyrazolone derivative with anti-inflammatory, analgesic and antipyretic effects that is commonly commercialized in tablet form [2]. The new medicated form can assure a faster delivery and adsorption of the active ingredient.

In this study, sodium alginate and kappa-carrageenan were used alongside gelatine in order to obtain hydrogels containing propyphenazone with the aim to evaluate the release of the active ingredient at different stages of ingestion [3]. A particular part of this study is focused on observing the interaction between the components of the hydrogels and how each stage of preparation influences the stability of the material.

The prepared hydrogels were analysed by using different techniques, such as FTIR, thermogravimetric analysis, UV-Vis and electron microscopy (SEM).

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P8
STUDY OF POLYMER-BASED JELLIES FOR ANTIPYRETIC AND ANALGESIC DRUG

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The commonly used forms of medication are tablets, as they are safe and effective. People with dysphagia and children have difficulty swallowing them. For this reason, our research group has developed medicinal jellies with antipyretic and analgesic active ingredients [1]. Propyphenazone is a pyrazolone derivative with anti-inflammatory, analgesic and antipyretic effects [2]. Medicated jellies contain propyphenazone, preservatives, gelling agents, stabilisers, and sweeteners.

In the synthesis of oral medicated jellies, the gelling agent can be used alone or in combination to achieve different gelling effects. The different types of polymers that can be used in oral medicated jellies include gelatin, sodium alginate, carrageenan and cellulose derivatives [1].

Marine polysaccharides with various biological properties such as carrageenan, alginate or chitosan enable the discovery of new pharmaceutical formulations or active ingredients suitable for biomedical applications [3].

Our current study aims to develop a new pharmaceutical formulation to follow up the previous study based on a different dosage form with active ingredient containing marine polysaccharides.

The jellies prepared, based on different marine polysaccharides, were analysed by FTIR, thermogravimetric analysis, UV-Vis and electron microscopy (SEM) coupled with EDX.

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P9
COMPARISON OF THE BIOLOGICAL ACTIVITY OF THE ARILS, SEEDS AND MIXTURE OF TAXUS BACCATA

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Species of the genus *Taxus* are very long-lived trees of the gymnosperm group. The popularity of *Taxus* species is due to the discovery of diterpene alkaloids present in the bark and leaves, used as precursors in the synthesis and semi-synthesis of anticancer drugs, which are successfully used in the treatment of various types of cancer and are even on the World Health Organization (WHO) list of essential medicines [1,2].

This study aims to obtain extracts from the arils, seeds, and a mixture of seeds and arils of *Taxus baccata*, following the optimization of the extraction process to maximize the yield of biologically active compounds. We sought to compare the characteristics of each extract, as it is well-known that the aril of *Taxus* species is considered the only non-toxic part of the plant, while the other parts are toxic due to their potent alkaloid composition.

Physico-chemical characterization of the ethanolic extracts was performed using appropriate techniques, including:

FT-IR spectroscopy: to identify the key functional groups of the organic molecules present in the extracts.

Thermal analysis (TG-DTG): to investigate the thermal behavior of the extracts, assessing the stability of the compounds with respect to temperature variations. This is essential to prevent the degradation of biologically active compounds during further processing for pharmaceutical formulations, which will subsequently be tested both in vivo and in vitro.

In conclusion, species of the genus Taxus, known for their longevity and medicinal potential, are significant for their diterpene alkaloids, which serve as precursors in anticancer drug synthesis. This study focuses on optimizing the extraction process from Taxus baccata arils and seeds to maximize biologically active compounds. The physico-chemical characterization of these extracts, using FT-IR spectroscopy and thermal analysis, provides insights into their functional group composition and thermal stability, which are crucial for developing pharmaceutical formulations without degrading the bioactive compounds.

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P10
PHYSICOCHEMICAL AND ANTIOXIDANT CHARACTERISATION OF A FOOD SUPPLEMENT BASED ON GINGER (*Zingiber officinale)*, IN VITRO EVALUATION

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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].

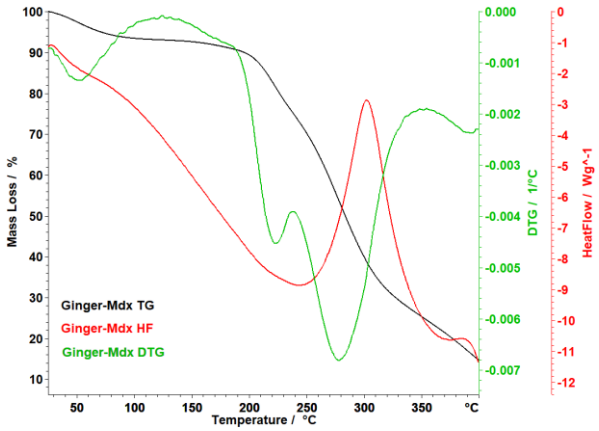

Figure 1. Thermoanalytical curves of Ginger-Mdx

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P11
INSIGHT INTO THE PHYSICOCHEMICAL AND THERMAL BEHAVIOR OF NEW MICROCARRIERS BASED ON ROMANIAN WILD-GROWING *Inonotus obliquus*

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Abstract

Chaga mushroom (*Inonotus obliquus*) is a fungus known for its therapeutic properties in traditional medicine [1-2].

Recent research has been focusing on its chemical composition and biological activity. The proportion of phytoconstituents varies due to various endo and exogenic factors, including the host tree (birch), as it is a pathogenic plant [1-2]. The maltodextrin microencapsulation of bioactive compounds is a popular method to enhance their stability and release mechanism [3].

This study presents the two spray-dried maltodextrin microcarriers based on Romanian Chaga mushroom preparation The first microcarrier emerges from Chaga microencapsulation in maltodextrin. The second carrier was prepared in two successive stages, namely Chaga-AgNPs complex formation and accompanied by the new complex microencapsulation in maltodextrin.

The morpho-structural and thermal behavior of the newly prepared microcarriers were analyzed using several techniques, including FT-IR, XRD, DLS, SEM, EDS, Raman, and thermogravimetric analysis.

The collective results demonstrate the preparation of the new microcarriers. Additionally, microencapsulation in the maltodextrin matrix increased the thermal stability of carrier systems.

Further studies will address the biological activity of both microcarriers.

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Functional Materials, Ceramics, Metals & Alloys, Cements and Engineering Materials & Composites

P12

EXPERIMENTAL RESEARCH ON THERMAL-ELECTRICAL BEHAVIOUR OF LANTHANUM MANGANITE COMPOUNDS

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Metal oxides with perovskite structure represent an important class of materials due to their electrical, mechanical, optical, magnetic and catalytic outstanding properties [1]. Moreover, because of their architectural, thermal durability, ionic conductivity and catalytic qualities, perovskite oxide substance has attracted a lot of interest for use in a wide range of fields, such as gas detecting, fuel cells, visible light photo-catalysis, magnetic memory devices, photovoltaic cells, metal-air batteries, and pseudo-capacitors [2].

This work has examined the impact of dopants on the physico-chemical properties of lanthanum manganite compounds which have been synthesized via sol-gel technique, and thermal treated at low temperature. Crystalline parameters of the as-prepared samples were analysed by X-ray Diffraction studies (XRD). Fourier transform infrared (FT-IR) measurements are utilized to detect the functional groups present in the sample. The shape and elemental content of the obtained nanomaterials were determined using scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDX). Thus, we have studied the structural, thermal and electrical properties of undoped and Ga or Y doped lanthanum manganite, in its R-3c space group (pristine sample) and Pm-3m space group (Y and Ga doped lanthanum manganite). The thermal analysis performed in the atmosphere of synthetic air in the range 25-900 ℃ revealed a different behaviour of the samples, namely in the case of the undoped sample there is a mass loss of 2.13% of the sample mass in the range 25-689 ℃ and then a mass loss of 0.2% in the range 690-820 ℃. Also in this last interval, an exothermic process with an $\Delta H = -29.48\ J \cdot g^{-1}$ is observed on the HF curve. In the case of the Ga doped $LaMnO_3$ material, a mass loss of 5.11% of the sample mass is observed in the range of 25-600 ℃ and a mass loss of 2.8% over 600 ℃. The quantitative analysis of the obtained materials demonstrates that the samples are with the expected elemental composition. The stoichiometry of the obtained samples was confirmed by the quantification of the elemental atomic ratio La:Mn:O i.e., 1:1:3. Thus, a homogeneous distribution of the corresponding La, Mn, O, Ga/Y elements in the synthesized samples was observed.

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P13
USING OF THERMAL METHODS TO IDENTIFY FUNCTIONAL GROUPS ON THE ACTIVATED CARBONS SURFACE

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The purpose of this work was the determination of the functional groups on the surface of activated carbons (AC) by temperature programmed decomposition method with mass spectrometric detection (TPD-MS) and thermal analysis (TA). Through these methods, the functional groups and the species adsorbed on the surface of the activated carbons can be determined (carboxylic acids, lactones, anhydrides, phenolic groups, carbonyl and quinones groups, etc.) [1, 2].

This paper discusses thermal analysis (TA) and TPD-MS characterization of several types of activated carbon, from walnut shell: (CAN - obtained by physical chemical activation method, CAN-Cl - modified with chloride ions, CAN-7 - obtained by chemical activation with phosphoric acid method) and pit coal: (AG-5 - commercial available and AG-5ox – oxidized with nitric acid).

The thermal stability of activated carbons was evaluated by the thermogravimetric method. A slow decrease in the mass of the CAN sample was observed with the increase of the temperature up to 450°C, which is due to the elimination of water and some volatile species from the structure of the activated carbon. At temperatures higher than approx. 450°C activated carbon burns. After the modification with chlorine ions, the activated carbon sample CAN-Cl becomes more thermally unstable. The temperature (430-440°C) at which the sample mass decreases is influenced by the chlorine ions present on the surface of the activated carbon. For AG-5 and AG-5ox activated carbons, an initial mass loss is observed at a temperature of approx. 100°C. After 450°C, the behavior is the same as for the activated carbons CAN and CAN-Cl. The mass spectra of the activated carbons samples CAN, CAN-Cl, AG-5, AG-5ox and CAN-7 reveal that at the temperature lower than 400°C, the most unstable functional groups are decomposed and eliminated as CO_2, which reveals the presence of carboxylic functional groups on the surface. The CO released from presented above, active carbons beyond 600°C shows the presence of phenolic groups, carbonyl groups and quinones. Meanwhile, the elimination of C_2H_6 and CH_4 from the samples CAN and CAN-Cl, suggests on the uncompleted (partial) activation of the activated carbon.

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P14
THERMAL ANALYSIS INVESTIGATION OF REGENERATED SATURATED PHENOL SATURATED ADSORBENTS

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One of the substances that is most hazardous and carcinogenic to both living things and the environment is phenolic compounds [1-3]. Large specific surface area, chemical and thermal stability MOF, and ease of synthesis are the major characteristics needed for adsorbent materials [2,3]. Ionic liquid (IL) based on imidazolium was utilized to functionalize a metal organic framework (MOF) based on a bisphosphonate with bivalent cations, which was then employed as an adsorbent for phenol (PH). Saturated MOF-IL adsorbent recovery was carried out by electrochemical oxidation (EO). One key finding that indicates the possible use of treated adsorbents for wastewater treatment is their regeneration and reuse. ATR-FTIR and TG analysis was done to examine the stability of the adsorbent following regeneration. The P-OH acid group's distinctive bands present in phosphoric acids are present in all spectra. The broad band seen in the FTIR spectroscopic study of at 3400–3500 cm^{-1}, is consistent with the TGA diagrams and indicates the water coordination molecules in the sample component. The initial mass loss of around 3.5% up to 105°C, represents the adsorbents' solvent trace and humidity elimination. The loss of coordinated water molecules accounts for the second major weight loss, which occurs in the temperature range of 110–250 °C. The quantity of coordinated water molecules is determined by both the cation's nature and the existence of IL nature. This is a two-step process wherein the water content of the crystallization molecules decreases gradually. The coordinated water loss was about 13.5%. The third major loss occurs in the temperature range of 250–400°C, where adsorbent lose about 7.8% of its weight. This loss coincides with the start of the metal-organic network breakdown. Thermal breakdown takes place above 400 °C. During the process of adsorption-desorption, the mass of the adsorbent remained unchanged. The electrooxidation doesn't lead to the collapse of the framework, and the adsorbent can be reused further.

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P15
EVALUATION OF TWO MATERIALS AS ADSORBENTS FOR THE REMOVAL OF PHENOLIC DERIVATIVES FROM WATER

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The growth and development of the industry means that organic pollutants, such as phenol and phenol derivatives, can be found in water, affecting the quality of life and the environment. Because of their solubility, these pollutants are difficult to remove from water, and the costs are extremely high. Therefore, we need materials that can adsorb these pollutants that are low-cost, reusable, and have minimal or no toxic effects on the environment. The aim of this work is to synthesize different solid materials, taking into account the 12 principles of green chemistry, obtaining materials with high adsorption capacities for phenolic derivatives.

The phosphonic metal-organic frameworks were obtained from the reaction of etidronic acid (HEDP)- as the organic linker, with divalent metal salts (Co^{2+}, Mg^{2+})- as the inorganic component, under hydrothermal conditions [1], using water as solvent. The next step in the synthesis was the impregnation of the materials with imidazole-based ionic liquids, specifically 1-ethyl-3-methylimidazole chloride, to increase the adsorption capacity, resulting in IL@MOFs. The adsorption of phenol derivatives (2,6-dimethylphenol) was tested, and it was found that the ionic liquid impregnated materials had a higher adsorption capacity compared to non-impregnated ones. CoHEDP yielded the best result, with a maximum value of 16.9 mg/g for 2,6-dimethylphenol [2].

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P16
SYNTHESIS AND CHARACTERIZATION OF SOME COMPOUNDS ORGANO-METALLICS BASED ON PHOSPHORUS

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Organometallic phosphorus compounds are of great interest due to their varied applications in catalysis, medicine, and advanced materials. These compounds exhibit diverse structures and properties, which are influenced by the nature of the organophosphorus ligand and the central metal. In this paper, we will explore the synthesis and characterization of organometallic compounds with phosphorus, more specifically organometallic compounds with aluminum and iron as central metals and 2-carboxy-ethyl phenyl phosphinic acid as ligand. Ethanol and N,N'-dimethylformamide are the chosen solvents for this work, and the method used is hydrothermal. The FTIR analysis was carried out using the FTIR Spectrophotometer Shimadzu IRTracer100, ATR technique (se fig. 1), in the range 4000-400 cm^{-1}, resolution 4 cm^{-1}, 10 repetitions for each sample and the thermoanalytical curves were obtained using a Mettler TOLEDO TG/DSC3+ analyzer in current of synthetic air (5.0) in the temperature range 25-400 °C (see fig. 2), with a speed of heating at 10 °C/min in aluminum crucibles followed by DSC study.

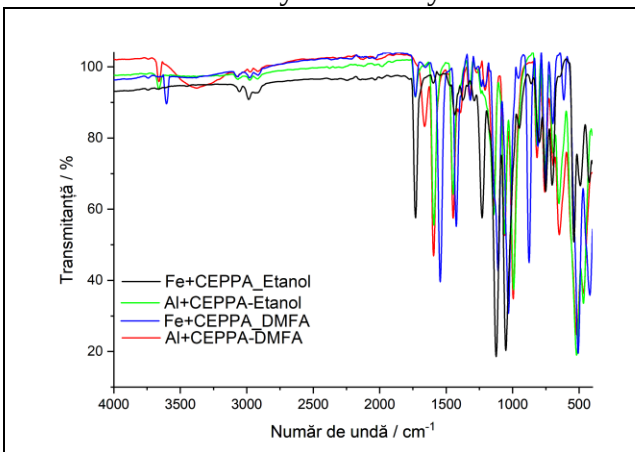

Fig. 1. Comparative FTIR spectra of sample obtained in different solvents

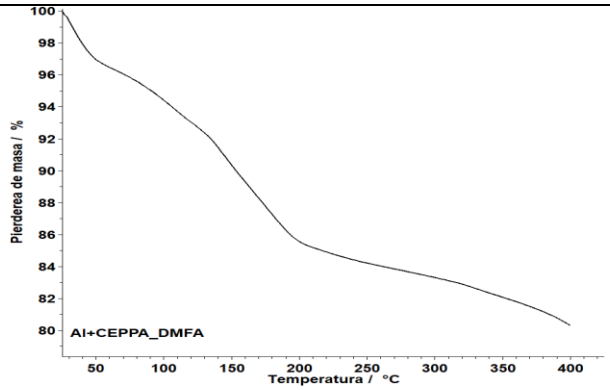

Fig. 2. TG/DTA analysis of the combination with Al in DMFA

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P17
IMMOBILIZATION OF ENZYMES ON CHITOSAN HYDROGELS – SYNTHESIS, PROPERTIES AND APPLICATIONS

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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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P18
EXPLORING THE POTENTIAL OF BLACK LIQUOR AS A REINFORCING AGENT FOR MODERN ADOBE BRICK COMPOSITES

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Throughout history, earth has often been used as a construction material for urban and rural houses in Romania[1]. In the Banat region, one of the most widespread ways of construction was using adobe bricks, obtained by mixing local earth (which contains clay), water, and shredded straw, then molded into a rectangular shape and air-dried[2]. Black liquor is an aqueous solution comprised of lignin and hemicellulose residues and the inorganic chemicals used in the kraft pulping process[3]. As reported in the literature, the viability of lignin as a chemical additive to treat geomaterials has generated promising results, especially in the improved properties of lignin-stabilized clayey soils and silty sands[4].

The main objective of the present study was to explore the potential of black liquor as a reinforcing agent for adobe brick, aiming to obtain composites with improved mechanical properties. These composites could help reduce the environmental issues caused by black liquor disposal, proving that turning waste into valuable resources is an important step towards sustainability in construction industries.

The resulting composite samples were analysed through thermogravimetric analysis, SEM, and FTIR analysis, while the influence of black liquor on their mechanical properties, namely compression and flexural strength, in accordance with EN 1015-11 [5] testing methodology.

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Heritage and Archaeological study

P19

THE STUDY OF RED PIGMENTS IN POWDER FORM AND MIXED WITH BINDERS USING PHYSICAL AND CHEMICAL INVESTIGATIONS

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The following study presents a multianalytical approach for the characterization of pictorial surfaces containing blue and red pigment.
The preliminary scientific investigations which include thermal and spectroscopic analysis are corroborated with the examination of the state of preservation of the color film belonging to a painting on glass from the 19th century.
The post-execution investigation included the correlation of scientific investigation data with the observation and interpretation of images obtained by optical microscopy. For the evaluation of the behavior of the pigments that are the subject of this study, a set of 7 pigments (Vermilion imitative divolo, Permanent red, Carminrot studienpigment, Burnt Siena, Iron oxide red, Cadmiumrot no.3, Universal red) and 37 mixtures with organic binders were analysed. For the organic binders, solutions of: rabbit glue, lean egg yolk emulsion, ox gall, boiled linseed oil, oil- in- water emulsion (linseed oil, egg yolk and lavender oil) were prepared and tested. The pigment-binder samples were applied to the glass support.
The distinct parameters observed under the digital microscope were the following: color - in the VIS spectrum and surface morphology in relation to the interaction of the binder.
The chosen case study is part of the painting category, representing an icon made in the traditional tempera technique with egg yolk emulsion on a glass support. The representation is included in the register of traditional glass painting from the Transylvanian area, with the iconographic theme, "The Birth of Jesus Christ", a common theme for Christian iconography. The support has a double role as both a support and a protective layer, the color film being applied to the back of the manufactured glass.
Microscopic analysis revealed the following forms of degradation of the pictorial layer: massive detachment from the support, scaling, decohension, drying and aging cracks, dehydration of the painting layer, lacunae, discoloration of the pigment, chemical alteration of the pigment in the form of chromatic modification, adherent and non-adherent deposits of organic and anorganic matter - dust, dirt, sand, greasy matter, insects of various species.

P20
A COMPARATIVE STUDY BETWEEN BLUE PIGMENTS FROM ORIGINAL PAINTING LAYERS AND CONTEMPORARY REPLICAS

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This paper aims to summarize the results of color film analysis in comparison with visual observation performed with a portable digital microscope, measurement of color coordinates and interpretation of spectra for the identification of pigments and their mixtures with different binders. The purpose of this research is to compare the data results from the created samples, to the study of the blue pigment found in a deteriorated state, as a constituent part of the original polychromy of the tempera painting on a wooden support: the icon of the Saint Archangel Gavriil. The main objective of the endevour is the selection of a consolidant with compatible visual and physico-chemical properties, for ensuring an adequate treatment for the particularities of polychromy.
The degradation of the pigment is directly related to the poor state of conservation of the entire work, affected by the cohesion and adhesion instability of the binder in the preparation layer, but also the decohesion of the color binder. The characteristics of the pictorial layer are the dullness of the colors, the lack of an obvious protective layer, and the mass dehydration of the entire structure. A particular problem with blue pigment is its discoloration in decohesive areas and local color change in background areas.
Through the replicas, the characteristics of the studied pigment were observed under the optical microscope, through the comparative analysis of the pigment in the state not degraded by the mixture with the selected binders. The replica set includes a repertoire of 77 mixtures of 10 blue pigments (Ultramarin ghiaro, Ultramarin Blue deep, True blue medium, Turquoise dark, Sky Blue, prod. Deifel, Manganblau, prod. Deifel, Echtblau kalfarbe= Real blue lime paint, prod. Deifel, Prussian blue, prod. Schmincke, prod. Schmincke) together with organic binders, prod. Deifel, Clei iepure, prod. CTS, pure hydrolyzed collagen, prod. Swedesh Collagen, Fu- nori japonisscher Algenleim, prod. Kremer, Aquazol ® 500, prod. Kremer, Paraloid B72, prod. CTS, Gum arabic, prod. Schincke, Egg Yolk Emulsion

P21
THERMAL AND HYPHENATED TECHNICS IN THE STUDY OF PIGMENTS USED IN PAINTINGS

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Colours are an essential part of human civilization since ancient times. People started to search for natural sources of colours and found out that some grounds, plants, insects can be smashed in powder form and be used to paint. These forms of colours are found under the name of pigments or dyes [1]. ***Pigments*** are ones of the most important components present in different works of art, archaeological and heritage items. Meanwhile, the methods of obtaining and synthesizing them have evolved a lot, the number, but also the quality of these pigments increasing considerably [2-3].

This paper presents a more thorough study of some important and, among the most used and indispensable types of blue pigments. Ten shades from this category of pigments were chosen to be characterized both thermally and structurally. The pigments were both inorganic (*Ultramarine Ghiaro, Ultramarine Blue Deep, Turquoise dark, Manganese blue, Prussian blue*) and organic (*True blue medium, Sky blue, Real blue, Phthalo blue, Indigo blue*) forms.

Different techniques as TG, DSC, SEM-EDX, FT-IR, also FT-IR microscopy etc., have been used to characterize the samples, for determination of their chemical structure and, also to lay the foundations for the creation of a new databases for their use in the restoration or authentication fields of various heritage items.

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P22
STATISTICAL ANALYSIS OF HERITAGE OBJECTS DATA ACQUIRED BY PHYSICO-CHEMICAL TECHNIQUES

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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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P23
Soil phosphate analysis of archaeological soil from Arad county

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Soils and archaeological deposits can be considered cultural artifacts, as they reflect the cultural environment in which they were formed. The study of these materials is the key to understand past agricultural and archaeological activities. Among the chemical elements that can provide clues for recognizing and locating sites of past human habitation, phosphorus stands out as the most chemically stable. In addition, it is easy to investigate both in the laboratory and in the field [1]. The high amounts of phosphates in the soil are an obvious indicator that the former inhabitants probably used the area for the disposal of waste with a high organic matter content, originating from human addition of manure from stables, food scraps, animal remains, etc. [2].

In order to study the anthropogenic soil of an archaeological complex in Arad county, ten sediment samples were collected from site no. 5 (outside the city of Arad, Arad county), located on the left bank of the Mures river, after the protection barrage. The samples were collected from key points of an archaeological survey. The phosphorus content of the samples was determined spectrophotometrically at 830 nm, according to Romanian standard, STAS 12205-84. The structure and properties of the soil samples were analysed using Fourier transform infrared spectroscopy (FT-IR), thermogravimetry and scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM-EDX). The phosphorus content of the samples ranged from 50 to 377 mg P/kg soil. FTIR spectra showed the characteristic bands of PO_4^{3-} (at 1090-1032, 960 and 600-500 cm^{-1}). From the SEM images it can be observed that the particles have different sizes and morphology, sharp, flat or spherical, with low porosity. Experimental results confirm that the soils of the archaeological site show traces of anthropogenic activity.

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P24

THE USE OF MULTIPLE TECHNIQUES IN THE INVESTIGATION OF SOME FRAGMENTS OF DACIAN CERAMICS, DISCOVERED NEAR THE DACIAN FORTRESS OF ALUN-PIATRA ROȘIE (HUNEDOARA COUNTY)

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The 16 samples presented in this work come from the research carried out on the surface of a terrace arranged on the southern slope of the Piatra Roșie hill, in the village of Alun, Boșorod commune, Hunedoara county, Romania. In that place, a construction made of wood was identified, on the surface of the ground, having the appearance of a household. The vessel fragments come from containers specific to Dacian pottery. The archaeological literature recorded the results of research, as well as some isolated discoveries, in the form of a monograph [1] and several studies, larger or smaller in size [2].

The analysis was conducted using complementary techniques TG/DTA, FT-IR (Figure 1), XRD, SEM-EDS, XPS, X-ray Computed Tomography (XCT) (Figure 2) and high-performance micro-focus X-ray, in order to determine details regarding production technology and origin of the raw materials.

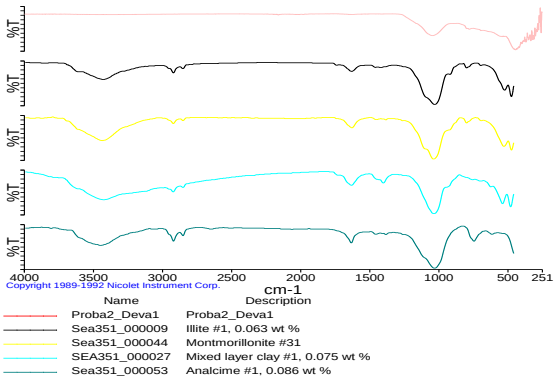
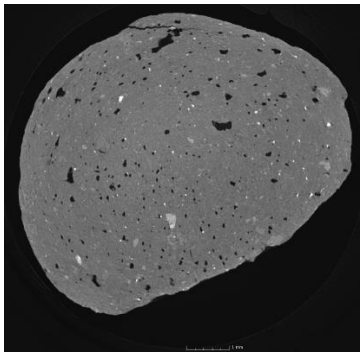


Figure 1. FT-IR sample 2



Top view
Inclusions of up to couple of tens of microns (bright spots) and pores up to couple of hundredts microns (black holes)

Figure 2. Microtomography cross-sections of Sample 2

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P25

BRONZE, FAIANCE AND UNKNOWN: ANALYSIS OF LATE BRONZE AGE SAMPLES FROM THE *GRĂMURADA DE LA JUPANI* SITE (SUSANI, TRAIAN VUIA, TIMIS COUNTY, ROMANIA) USING HYPHENATED TECHNIQUES

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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 parrish, 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 and thermal analysis (TMA), in order to identify composition and manufacturing technique [2-3].

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P26

BEYOND THE MOUNTAINS: ANALYSIS OF BRONZE AGE POTTERY SAMPLES FROM THE VÂNĂTORI-NEAMȚ - *VALEA REA* FORTIFICATION (VÂNĂTORI-NEAMȚ, NEAMȚ COUNTY, ROMANIA) USING MULTIPLE ANALITIC TECHNIQUES

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The analyzed objects are from the Vânători-Neamț – „Valea Rea" fortification on the western side of the Neamț Depression, near the Vânători-Neamț (Neamț county, Romania), discovered in 2020. Archaeological excavations started in 2021 and still ongoing. The site occupies a small wooded triangular plateau, with a relative height of 6 m above the surrounding area, on the right bank of the Neamț river, situated near the begining of the highlands. A sample taken from the site's southern area, from a likely defensive ditch, allowed the dating of the feature to cca. 3039-2892 calBC [1].

The samples were taken from 12 pottery sherds, covering coarse and semifine ceramics specific to the site. As physical-chemical analysis was not performed (to date) on Bronze Age pottery from the Eastern side of the Carpathians, complementary techniques were used in the analysis (TG/DTG, FT-IR, SEM, EDX, XRF, XRD and LIBS) to ascertain details regarding production technology and composition, [2-4].

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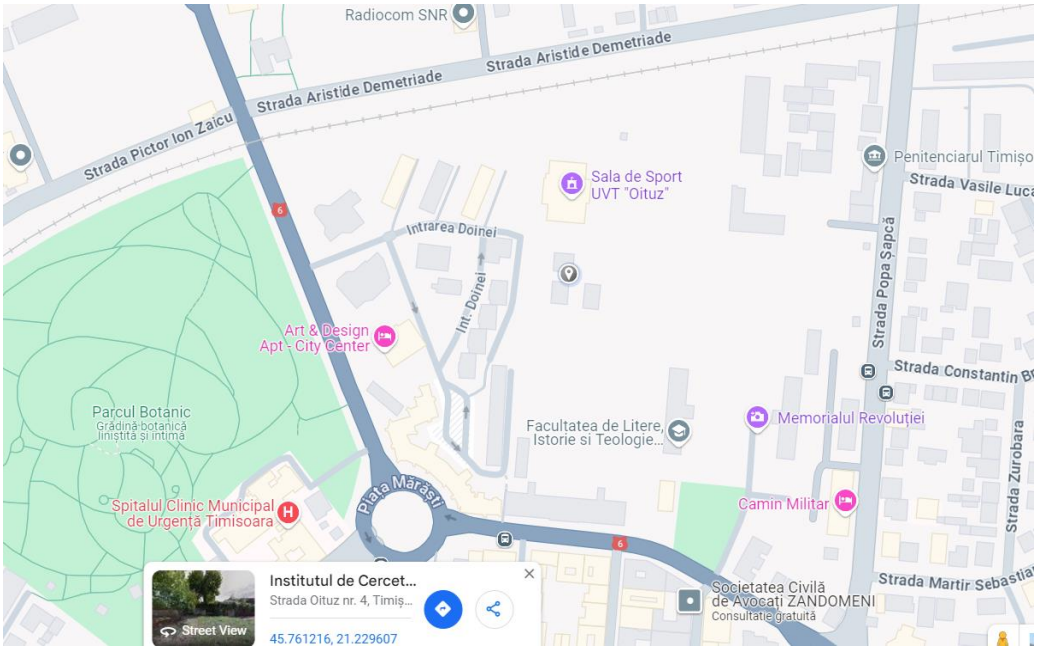

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