31st Symposium on Thermal Analysis and Calorimetry "Eugen Segal" of the Commission for Thermal Analysis and Calorimetry of the Romanian Academy

CATCAR31

20-22 October 2022, Reşiţa – Romania

UNIVERSITATEA BABEŞ-BOLYAI
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PROGRAM

Thursday, 20th of October 2022

18^{00}-19^{30}

18^{00}-18^{20}

Welcome to CATCAR31

Andrei Rotaru, Cornel Haţiegan

Chairpersons of CATCAR31

Topical trends in Thermal Analysis and Calorimetry 2018-2023

Andrei Rotaru

President of CATCAR

Session 1

Chairperson: Ionuţ Ledeţi

18^{20}-19^{00}

Plenary Lecture 1

Advanced isoconversional kinetic analysis combined with model-fitting applied to polymerization kinetics

Nicolas Sbirrazzuoli

University Côte d'Azur, France

19^{00}-19^{30}

Invited Lecture 1

Hybrid and composite oxide and carbon nanofluids

Imre Miklos Szilagyi

Budapest University of Technology and Economics, Hungary

20^{00}-23^{00}

Conference Dinner

Friday, 21st of October 2022

10^{00}-18^{30}

Session 2
Chairperson: Stefano Vecchio Ciprioti

10^{00}-10^{30}
Invited Lecture 2
Implementation of thermoanalytical techniques in investigation of pharmaceuticals

Ionuţ Ledeţi
University of Medicine and Pharmacy "Victor Babeş", Romania

10^{30}-10^{50}
Oral Presentation 1
Thermal behaviour of S–IPNs based on DGEBA and an oligophosponate

Cristian-Dragoş Varganici
"Petru Poni" Institute of Macromolecular Chemistry, Romania

10^{50}-11^{10}
Oral Presentation 2
The effect of temperature changes on the natural frequencies of a double-clamped prismatic beam

Gilbert-Rainer Gillich
Babeş-Bolyai University, Romania

11^{10}-11^{40}
Invited Lecture 3
Characterization of the thermal decomposition of $BaCO_3$ in YBCO precursor films

Jordi Farjas
University of Girona, Catalonia, Spain

11^{40}-13^{00}
Poster Session 1 & Coffee Break 1

13^{00}-14^{30}

Lunch break

Session 3

Chairperson: Jordi Farjas

14^{30}-15^{10}

Plenary Lecture 2

General rate equation and meaning of kinetic parameters

Peter Šimon

Slovak University of Technology, Slovakia

15^{10}-15^{30}

Oral Presentation 3

Case study on the methane gas explosion effects on civil buildings

Florin Manea[1,2]

[1]National Institute for Research and Development for Min Safety and Protection, Romania

[2]West University of Timisoara, Romania

15^{30}-15^{50}

Oral Presentation 4

Encapsulation of artemisinin and its derivatives by sulfobutylated β-cyclodextrin: physicochemical and molecular modelling studies

Amalia Ridichie

University of Medicine and Pharmacy "Victor Babeş", Romania

15^{50}-16^{20}

Invited Lecture 4

In search of the most convincing parameter to assess the thermal stability of materials

Stefano Vecchio Ciprioti

Sapienza University of Rome, Italy

16^{20}-17^{50}

Poster Session 2 & Coffee Break 2

Session 4
Chairperson: Cornel Haţiegan

17^{50}-18^{10}
Oral Presentation 5
Binary systems containing carvedilol

Bianca Bîrzava-Milu
University of Medicine and Pharmacy "Victor Babeş", Romania

18^{10}-18^{30}
Oral Presentation 6
Current approaches for methods and methodologies in heterogeneous kinetics

Andrei Rotaru[1,2]
[1]University of Craiova, Romania
[2]Institute of Physical Chemistry "Ilie Murgulescu", Romania

Saturday, 22nd of October 2022

10^{00}-12^{00}

Session Chairperson: Peter Šimon

10^{00}-12^{00}
Perspectives of Thermoanalytical Kinetics

12^{00}
Closing ceremony

POSTER SESSION 1

Poster Presentation 1

Thermo-physical aspects of the behaviour of some chloro-azomonoethers

Vily Cimpoiaşu
University of Craiova, Romania

Poster Presentation 2

The determination of the hydro-generator efficiency through the calorimetric method

Cornel Haţiegan
Babeş-Bolyai University, Romania

Poster Presentation 3

Determining the stability of the power transformer insulation at high temperatures

Cornel Haţiegan
Babeş-Bolyai University, Romania

Poster Presentation 4

Thermal behaviour of a coating based on epoxy resin and castor oil

Liliana Roşu
"Petru Poni" Institute of Macromolecular Chemistry, Romania

Poster Presentation 5

Pottery samples from the settlements and burial ground at Pecica – East site (Pecica, Arad County, Romania): analysis through hyphenated techniques

Gabriela Ursuţ
West University of Timişoara, Romania

Poster Presentation 6

Polysaccharide membranes as a delivery agent for local anesthetic drugs

Dorinel Okolišan
West University of Timişoara, Romania

Poster Presentation 7

Pottery and clay samples from the Neo-Aeneolithic settlement Şoimuş - Avicola site/ Şoimuş - Teleghi (Șoimuș, Hunedoara County, Romania): analyzed using hyphenated techniques

Gabriela Vlase
West University of Timişoara, Romania

Poster Presentation 8

Study of thermally induced interactions between active substances from the sartans class and various excipients

Titus Vlase
West University of Timişoara, Romania

Poster Presentation 9

Superionic Conductivity Modelling of NZSP NaSICON Synthesized by an Augmented SSR Method

Athanasios Tiliakos
National R&D Institute for Cryogenic and Isotopic Technologies (ICSI), Romania

POSTER SESSION 2

Poster Presentation 10

Synthesis and characterization of silver ion doped hydroxyapatite

Alexandra Tăşală
West University of Timişoara, Romania

Poster Presentation 11

The properties variation of hydroxyapatite dispersed into polymer matrix during thermal treatment

Alexandru Pahomi
West University of Timişoara, Romania

Poster Presentation 12

Coagulant – antibiotic scaffold systems for dental application

Mădălina Mateescu
West University of Timişoara, Romania

Poster Presentation 13

Composites with antibiotics, bisphosphonate and hydroxyapatite for dental applications

Mihaela Maria Budiul
West University of Timişoara, Romania

Poster Presentation 14

Kinetics of thermal degradation of pharma grade sulfobutylether sodium betacyclodextrin

Adriana Ledeţi
University of Medicine and Pharmacy "Victor Babeş", Romania

Poster Presentation 15

Instrumental investigations of telmisartan-aminoacids binary adducts

Bianca Baul
University of Medicine and Pharmacy "Victor Babeş", Romania

Poster Presentation 16

Heptakis(2,6-di-O-methyl)-β-cyclodextrin inclusion complex of olmesartan medoxomil. Compatibility with excipients

Laura Sbârcea
University of Medicine and Pharmacy "Victor Babeş", Romania

Poster Presentation 17

Transmucosal absorption of antibiotic-anesthetic polymer-based systems for dental use

Ionela-Amalia Bradu
West University of Timişoara, Romania

Poster Presentation 18

Theoretical and instrumental approach for the development of co-crystals with mirtazapine and opipramol

Denisa Cîrcioban
West University of Timişoara, Romania

***Conference address**:*
Piaţa Traian Vuia, Nr. 1 – 4, 320085, Reşiţa, Caraş-Severin, Romania
Faculty of Engineering, Block A, 2nd floor, Conference room

PLENARY LECTURES

Plenary Lecture 1

Advanced isoconversional kinetic analysis combined with model-fitting applied to polymerization kinetics

Nicolas SBIRRAZZUOLI

University Côte d'Azur, Institute of Chemistry of Nice, CNRS UMR 7272, France
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Advanced isoconversional kinetic analysis combined with model-fitting may provide new mechanistic interpretations, opening the door to new applications. Polymerizations are complex chemical reactions during which long macromolecular chains are produced from small monomer molecules, complicated by physical transformations such as gelation or vitrification. As consequence, during the later stages of the reaction, there is an interplay between the contributions of chemical reaction and diffusion step to the overall reaction rate, followed by a shift of the reaction from chemical to diffusion control. This is the result of the high increase of the molecular weight and viscosity due to crosslinking. Thus, extracting the kinetic parameters of each individual step for such complex processes is not straightforward.

The present work describes the polymerization kinetics and chemo-rheology of various systems, by coupling real-time ATR-FTIR, DSC data, heat capacity variations, rheometry, with isothermal and nonisothermal kinetics. New insights into the mechanisms of crosslinked network formation are provided. Two macro-kinetic models are proposed that accurately describes the experimental data and can account for both the chemically and diffusional controlled parts of the reaction, leading to kinetic parameters with real physical meaning [1-7].

[1] S. Vyazovkin, N. Sbirrazzuoli. Macromolecules, 29 (6) (1996) 1867-1873.
[2] A. Sangregorio, N. Guigo, E. de Jong, N. Sbirrazzuoli. Polymers, 11 (2019) 1804.
[3] C. Menager, N. Guigo, L. Vincent, N. Sbirrazzuoli. J. Polym. Sci., 58 (2020) 1-11.
[4] N. Sbirrazzuoli. Molecules, 24 (2019) 1683.
[5] N. Sbirrazzuoli. Thermochim. Acta, 691 (2020) 178707.
[6] N. Sbirrazzuoli. Polymers, 12 (2020) 1280.
[7] S. Vyazovkin, D. Achilias, X. Fernandez-Francos, A. Galukhin, N. Sbirrazzuoli. Thermochim. Acta, 714 (2022) 179243.

Plenary Lecture 2

General rate equation and meaning of kinetic parameters

Peter ŠIMON, Zuzana CIBULKOVÁ, Tibor DUBAJ
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Slovak University of Technology, Radlinského 9, 812 37, Bratislava, Slovakia,
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Processes in condensed phase are extensively studied by thermoanalytical methods. Mechanisms of these processes are very often unknown or too complicated to be characterised by a simple kinetic model. They tend to occur in multiple steps that have different rates. To describe their kinetics, the methods based on the single-step approximation are often used which are represented by the general rate equation [1]:

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} = k(T)\,f(\alpha) \tag{1}$$

where α is the degree of conversion of the process, t is time, T is temperature, $k(T)$ and $f(\alpha)$ stand for the temperature and conversion functions, respectively. It will be demonstrated that Eq. (1) is not a true kinetic equation and that it is just a mathematical tool for describing the kinetics of the process. The parameters in the temperature and conversion functions have unclear physical meaning in general; however, they enable to model the kinetics of the process.

The methods based on Eq. 1 can be divided into the model-free (or isoconversional) and model-fitting ones [1]. It will be shown that the integral isoconversional methods are mathematically incorrect and should not be applied. As for the model-fitting methods, a quite extensive list of conversion functions in Eq.(1) is employed. On the contrary, only the Arrhenius equation is applied as the temperature function. Since the temperature function is not the rate constant, it is not inevitable to be confined to the Arrhenius equation in the case of the temperature function and that other, non-Arrhenian temperature functions can be applied.

Acknowledgement
Financial support from the Scientific Grant Agency of the Slovak Republic (VEGA 1/0498/22) is greatly acknowledged.

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INVITED LECTURES

Invited Lecture 1

Hybrid and composite oxide and carbon nanofluids

Imre Miklós SZILÁGY, Marcell BOHUS, Zalán István VÁRADY, Thong LE BA

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In this lecture, the thermal conductivity and viscosity of various single phase, hybrid and composite oxide and carbon nanofluids are presented. As solid nanomaterials for single phase nanofluids, halloysite nanotubes, SiO_2 and TiO_2 nanoparticles, carbon nanospheres and carbon nanopowders were used. For hybrid nanofluids, SiO_2-TiO_2 were applied. For the first time, core/shell nanomaterials obtained by atomic layer deposition (ALD) were also tried to increase the thermal conductivity of nanofluids. Hence, SiO_2/TiO_2, carbon nanosphere/TiO_2, carbon nanopowder/TiO_2 core/shell nanoparticles were studied in nanofluids. The nanofluids were prepared different nanoparticle volume concentrations (0.5, 1.0 and 1.5 vol%) at five various temperatures (20, 30, 40, 50 and 60 °C). The hybrid nanofluids were better in performance compared to the single phase ones. However, the ALD prepared core/shell ones were even more beneficial, which opens up a new way to obtain novel, beyond the state-of-the-art nanofluids.

Invited Lecture 2

Implementation of thermoanalytical techniques in investigation of pharmaceuticals

Ionuţ LEDEŢI

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The discovery and development of new pharmaceutical formulations containing new active pharmaceutical ingredients (APIs) is a complex and essential process for improving the life quality of humans. The development of these pharmaceutical formulations is preceded by the preformulation studies, where the investigations of physicochemical characteristics of compounds or biological entities that are candidates for development into final products are carried out.

In order to ensure that the pharmaceutical formulations are optimised for their intended use, preformulation studies must be realised not only to evaluate the characteristics of active ingredients, but also for the excipients, and their possible interactions during processing [1].

In this lecture, the main research directions regarding the characterisation of pharmaceuticals in our research group is presented – including phase transitions of solids, kinetics of decomposition, shelf-life and aging of different pharmaceutical formulations, existence of solvates/polymorphs/pseudopolymorphs, compatibility with excipients, and as well formation of binary adducts and supramolecular structures (salts, cocrystals, inclusion complexes) [2-4].

[1] Jones, T.M. CHAPTER 1: Preformulation Studies. In RSC Drug Discovery Series; The Royal Society of Chemistry, 2018; Vol. 2018-January, pp. 1–20 ISBN 978-1-84973-941-2.
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[4] Ledeţi, I.; Vlase, G.; Vlase, T.; Fuliaş, A. J. Therm. Anal. Calorim. 2015, 121, 1103–1110.

Invited Lecture 3

Characterization of the thermal decomposition of $BaCO_3$ in YBCO precursor films

Sihem ZAIDI[1], Anna PLANELLA[1], Daniel SÁNCHEZ-RODRÍGUEZ[1], Lavinia SALTARELLI[2], Jordi FARJAS[1], Pere ROURA-GRABULOSA[1], Xavier OBRADORS[2], Teresa PUIG[2]

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The energy transition towards a drastic reduction of CO_2 emissions is one of most important challenges that humanity faces; by 2050 the use of renewable energy should account for 80 to100% of the total energy [1]. To this end, high temperature superconductivity (HTS) is identified as a crucial technology [2, 3]. In particular, $REBa_2Cu_3O_7$ (REBCO) coated conductors (CCs) are foreseen for a wide market implementation [4]. However, nowadays REBCO CCs are not competitive, so it is of utmost importance to reduce the manufacturing cost while achieving a high current density. Thus, new methodologies are required to synthetize in a single step thick films (beyond 1 μm) with a critical current density above 4 MA/cm2 at 77 K and at a high yield.

We have recently demonstrated that it is possible to growth YBCO films at fast rates as high as 100 nm/s through the so-called transient liquid assisted growth (TLAG) process [5]. TLAG is based on the eutectic reaction between $BaCuO_2$ and CuO to form a transient liquid in the region of the phase diagram where solid YBCO is the equilibrium phase. The fast atomic diffusion and high atomic density of the liquid phase with respect the solid phase allows to achieve ultrafast growth of YBCO. The limiting step for YBCO growth is the decomposition of $BaCO_3$. In this work we analyse the decomposition of $BaCO_3$ in the form of films and under the conditions to achieve the TLAG process. In particular, we analyse the effect of the presence of Cu and Y oxides, the presence of metastable $BaCO_3$ phases [6], the role of the film thickness on the kinetics as well as the composition of the surrounding atmosphere.

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[2] Shiohara Y, Taneda T and Yoshizumi M. J. Appl. Phys. 51 (2012) 010007
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[6] S. Rasi et al. J. Phys. Chem. C. 124 (2020) 15574–15584.

Invited Lecture 4

In search of the most convincing parameter to assess the thermal stability of materials

Stefano VECCHIO CIPRIOTI

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Information concerning the thermal stability of materials in the condensate state (mainly solid) is of paramount practical and technological importance [1]. Materials are usually characterized for testing them in several kinds of applications and assess their thermal stability since they may undergo fire accidents or may be stored in suitable places for a long time where temperature can increase, especially during the summer time. In other cases, they are thermally treated for their preparation (like for steel) or to enhance their mechanical properties. Lifetime prediction of cables in nuclear power plants is based on the isothermal simulation of their ageing at elevated temperature [2].

Three stability parameters related to the thermal decomposition of different classes of materials have been considered: onset decomposition temperature (T_{on}), activation energy of decomposition (E_a) and reaction rate ($k(T_{ref})$, determined according to the well-known Arrhenius equation at a given appropriate temperature T_{ref}). The first quantity is the most commonly used parameter to construct a relative stability scale among material undergoing the same degradation process (accompanied by the same reaction mechanism). Several examples regarding this parameter will be presented and critically discussed, but some limitations in assessing the stability scale could arise especially when the difference of T_{on} values are negligible, since many experimental operating conditions may affect the values obtained. Then, the activation energy was taken into account. Isoconversional model free methods were adopted and the results were interpreted in terms of the energy barrier that the reactants must overcome to cross the transition state and to obtain the products. Some examples will be presented and discussed, although the Compensation Effect, a linear relationship between E_a and $\ln A$ values avoids the use of this parameter for the claimed purpose.

Finally, since thermogravimetry (TG) is often adopted to study the kinetics of thermally activated solid-state reactions or thermal decompositions of liquids [3,4], it is suggested to process TG (or DTA or DSC data) to derive a kinetic parameter that combine Arrhenius pair aiming at assessing a more convincing thermal stability scale.

[1] S. Vyazovkin, "Isoconversional Kinetics of Thermally Stimulated Processes", Ed. Springer International Publishing Switzerland, (2015).

[2] M. Beneš, V. Plaček, G. Matuschek, K. Györyová, W. D. Emmerich, V. Balek, J. Therm. Anal. Calorim., 82 (2005) 761

[3] K. Chrissafis , K.M. Paraskevopoulos, D.N. Bikiaris. Polym. Degrad. Stabil.. 91 (2006) 60

[4] B. Tita, A. Fulias, E. Marian, D. Tita. Rev. Chim. (Bucuresti), 60 (2009) 419

ORAL PRESENTATIONS

Oral Presentation 1

Thermal behaviour of S–IPNs based on DGEBA and an oligophosponate

Cristian–Dragoș VARGANICI, Liliana ROȘU, Dan ROȘU
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Epoxy resins are known as a worldwide market dominating class of polymers, due to their versatile nature and relatively low cost. This aspect is due to the presence of the oxirane ring, capable of reacting with a variety of different compounds. This endows epoxy resins with excellent features, such as: good mechanical properties, adhesion to various substrates and resistance to corrosion, solvents and abrasion, etc. [1]. All these features recommend epoxy resins for a wide palette of applications: adhesives, circuit boards, engineering, construction, aeronautics, etc. Despite their excellent properties, epoxy resins are known of being highly flammable and with low thermal stability [2]. The improvement of these properties of the epoxy resins remains an important challenge to this day.

This study describes the obtaining of semi–interpenetrating polymer networks (S–IPNs) based on diglycidyl ether of bisphenol A (DGEBA) hardened with three different curing agents, aromatic, cycloaliphatic, and an aromatic oligophosphonate (OP) as linear component. The good miscibility of the OP in the cured DGEBA was demonstrated by DSC and morphological studies (SEM–EDX). The thermal stability of the S–IPNs was undertaken with TGA in nitrogen and air. The evolved gases analysis was conducted with TGA–FTIR and Py–GC–MS. A thermal degradation mechanism was proposed for the S–IPNs. The flame resistance of the S–IPNs was done via microscale cone calorimetry (MCC). The residual char obtained during the TGA was analysed by SEM–EDX. The obtained data showed that the S–IPNs possess both condensed and gas phase flame retardant mechanism.

[1] R. Thomas, P. Vijayan, S. Thomas, "Recycling of thermosetting polymers", Transworld Research Network, (2011) 122-129
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Oral Presentation 2

The effect of temperature changes on the natural frequencies of a double-clamped prismatic beam

Zeno-Iosif PRAISACH, Cristian TUFIŞI, Gilbert-Rainer GILLICH
Babes-Bolyai University, Str. Mihail Kogălniceanu, nr. 1, 400084, Cluj-Napoca, Romania

We analyze in this paper a beam clamped at both ends that is subjected to temperature changes. Because the beam ends are restrained, the temperature changes induce axial forces, having as a consequence the change of the dynamic behavior of the beam. The change consists of a natural frequency increase if the temperature of the structure becomes lower, and a drop if the temperature increases [1].

The finite element method (FEM) was involved to perform the thermal analysis. We tested the behavior of the beam in the temperature range of 0 to 125°C, the reference temperature being 24.85°C which is the default temperature for the SolidWorks - *Thermal analysis module*. and we derived the critical loads and temperatures for the first four buckling modes. The resulting values were compared with those calculated and we found a good fit.

Next, we introduce the critical loads in the equation that expresses the natural frequencies of the beam and obtain a mathematical relation that permits calculating the beam's natural frequencies in the case it is subjected to axial forces.

To test the validity of the contrived mathematical relation, we perform a modal analysis involving the FEM for different temperatures. The beam was analyzed by gradually changing the temperature. When decreasing the temperature a step of five Kelvin degrees was imposed, because the stretching forces generate a frequency increase by a phenomenon that is simple to be described. When increasing the temperature, buckling occurs and the frequencies decrease until reaching zero. This is a more complex behavior and therefore we considered a finer step of one Kelvin degree as necessary for a proper analysis. This helped us to precisely find the critical temperatures where the frequencies take the value zero, which should be the same as the critical buckling temperatures obtained from the static analysis [2,3]. We also compare the frequencies derived using the FEM with those calculated with the contrived relation and found two similar curves.

[1] A. Bokaian, Natural frequencies of beams under compressive axial loads, Journal of Sound and Vibation 126 (1988) 49-65.
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Oral Presentation 3

Case study on the methane gas explosion effects on civil buildings

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[2]West University of Timisoara, Timişoara, Romania

A tragic explosion[1] resulting from a methane gas leak occurred in the Christmas day in 2013, at an apartment building block with human losses and significant material damages. The investigation of the incident included physical determinations and CFD simulations of the explosion ignition, flame front propagation[2] and materials deformations in order to explain the destructive effects.

This paper will focus on the steps required to identify the critical conditions that led to the dynamic effects of almost 17 building apartments, 7 commercial building located at the building ground floor and even 14 cars from the building parking place. Based on the calculations, hypothesis and CFD[3] simulations the explosion ignition and propagation mechanism were elaborated strongly related to the onsite observations and criminal file issued by the state authorities.

[1] INSEMEX Colective, "'Investigation Report - specialized technical expertise of the event produced, on 25.12.2013, around 5:44 p.m., on Bucharest Street, no. 139, block A 38, sc. 2, floor 1, apartment 2 in Călăraşi municipality, Călăraşi county' – issued on May 2014.," Petrosani, 2014.

[2] O. D. Maria Prodan, Emilian Ghicioi, "CORRELATION OF EXPLOSION PARAMETERS AND EXPLOSION-TYPE EVENTS FOR PREVENTING ENVIRONMENTAL POLLUTION," *Environ. Eng. Manag. J.*, vol. 13, no. 6, pp. 1409–1414, 2014.

[3] A. B. Şimon-Marinică, N.-I. Vlasin, F. Manea, and G.-D. Florea, "Finite element method to solve engineering problems using ansys," *MATEC Web Conf.*, vol. 342, p. 01015, 2021, doi: 10.1051/matecconf/202134201015.

Oral Presentation 4

Encapsulation of artemisinin and its derivatives by sulfobutylated β-cyclodextrin: physicochemical and molecular modelling studies

Amalia RIDICHIE[1,2], Adriana LEDEŢI[2], Denisa CÎRCIOBAN[2], Gabriela VLASE[3], Titus VLASE[3], Renata VĂRUŢ[4], Francisc PETER[1], Ionuţ LEDEŢI[1,2]

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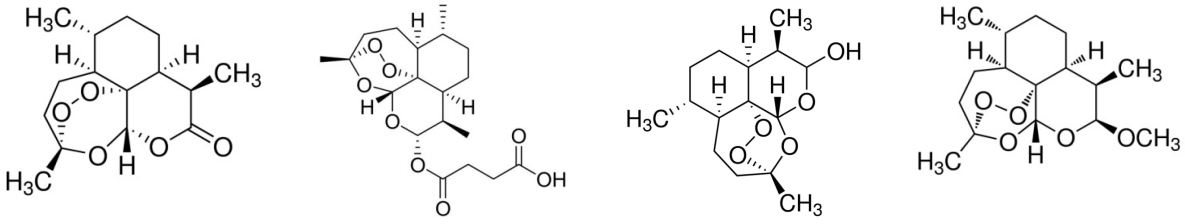
Keywords: solubility enhancement, inclusion complexes, artemisinin, thermal analysis

Artemisinin and several functionalised derivatives (artesunate, dihydroartemisinin, artemether, Figure 1) are commonly used in malaria therapy, while also having potent antitumor activity. However, they have low water solubility, belonging to BCS II class, so the improvement of biopharmaceutical profiles is possible by formation of inclusion complexes (IC) with cyclodextrins (CDs) [1,2].



(a) (b) (c) (d)

Figure 1. Structural formulas of artemisinin (a), artesunate (b), dihydroartemisinin (c) and artemether (d)

The purpose of this study was to prepare and characterise the ICs of these sesquiterpenes with a semisynthetic anionic cyclodextrin, namely sulfobutyl-ether-beta-cyclodextrin sodium salt (SBECD) using the wet kneading method. In solid state, the ICs were characterised by thermal methods (TG/DTG/HF), ATR-FTIR spectroscopy and PXRD profiles.

The results reveal different physicochemical properties of obtained ICs when compared with those of the drugs substances and cyclodextrin alone, demonstrating thus the formation of the supramolecular structures. Molecular modelling studies were carried out for an in-depth characterization of the interaction between artemisinin-type compounds and CD.

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Oral Presentation 5

Binary systems containing carvedilol

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Carvedilol (CARV, Figure 1) is a nonselective β-adrenergic blocking agent that is currently prescribed in the treatment of essential hypertension, angina pectoris and congestive heart failure. CARV belongs to the BCS II class, showing a low water solubility (0.583 mg/L1), but a highly permeability. Due to the low water solubility, the absorption is conditioned by the dissolution rate, resulting in insufficient and delayed absorption [1-3]. Due to this intrinsic profile of CARV, the search of methods for improving the dissolution profile is a challenge for scientists [1,3].

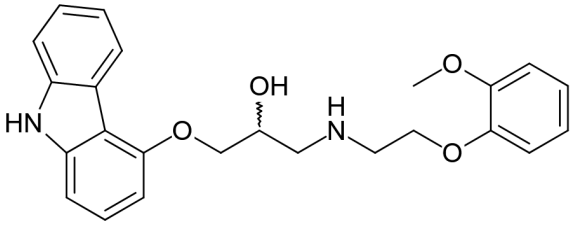

Figure 1. Chemical structure of CARV

In this study, binary mixtures containing CARV and several α-aminoacids (AA) were prepared using the kneading method by a known protocol [4], in molar ratios 1:1 and 2:1 CARV:AA and were characterised by FTIR spectroscopy and thermal analysis (TG/DTG/HF) in oxidative atmosphere. A discussion regarding the formation of adducts is also presented.

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Oral Presentation 6

Current approaches for methods and methodologies in heterogeneous kinetics

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Usually, the kinetic analysis of a heterogeneous process is performed under non-isothermal conditions, which are faster and cover a wider range of temperatures. The rate equation (eq. 1) may be separated into a term depending on the temperature, *k(T)* (commonly expressed by the Arrhenius equation) and respectively into the conversion function, *f(α)* (commonly expressed by various kinetic models or by the more general Šestak-Berggren model – eq. 2).

$$r = \frac{d\alpha}{dt} = k(T) \cdot f(\alpha) \tag{1}$$

where α is the conversion degree.

$$f(\alpha) = \alpha^{m}(1-\alpha)^{n}(-\ln(1-\alpha))^{p} \tag{2}$$

n, m, p are the kinetic model exponents.

Traditionally, the Arrhenius equation was employed for fulfilling *k(T)*, containing the activation energy, *E*, and also the frequency factor, *A*. Since many thermoanalytical techniques are recording integral data, and by differentiation procedure a high degree of noise is obtained, it was requested the development of integral methods. However, inexact integration produced big uncertainties, and there was always in the last 50 years a competition for the title of "best integral kinetic method", ultimately few advanced linear and non-linear methods were published. Here, we aim to find an efficient methodology based on the single heating rate equations (derived from Ortega and Tang & Chen methods), to be further employed not only as isoconversional methods, but also within the Invariant Kinetic Parameters (IKP) method and Perez-Maqueda *et al.* criterion.

On the other hand, the individual kinetic mechanisms that were derived during a much longer period of 100 years, benefited however of a historical "protection" and remained mostly untouched, even when the extended Šestak-Berggren model, encompassing few single models in a single expression has appeared. Unfortunately, although seeming to be a general expression that unifies, this extended model has some drawbacks, of which the most important is the impossibility to be exactly integrated and thus is no integral expression that may be used as part of integral kinetic methods. Therefore, it would be interesting to improve the mechanistic methodologies by making use of some novel theoretical aspects for the computation of some special class of integrals, and also to develop alternative ways to establish a better expression of the general conversion function by means of the control theory.

POSTER PRESENTATION

Poster Presentation 1

Thermo-physical aspects of the behaviour of some chloro-azomonoethers

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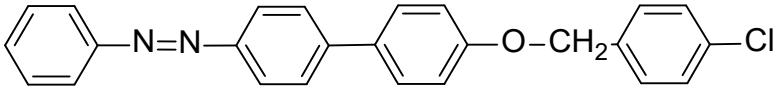
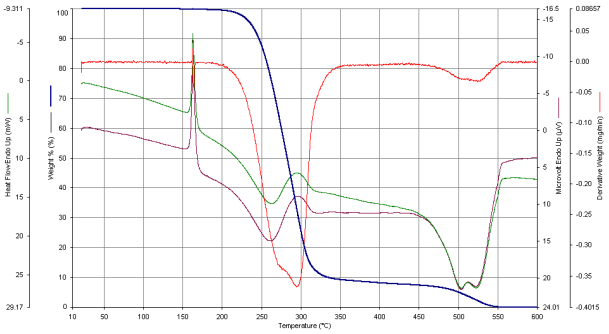
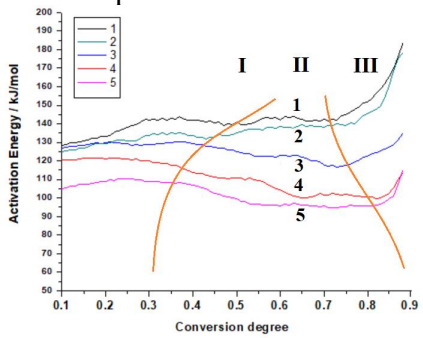
Five chloro-azomonoether derivatives of 1-(4'-((4-chlorobenzyl)oxy)-[1,1'-biphenyl]-4-yl)-2-phenyldiazene [1] were synthesized, with the structural formula:



using the condensation of different sodium salts of some 4'-phenyldiazenyl-biphenyl-4-ols with 1-chloro-4-(chloromethyl)benzene. The formation of azomonoethers was confirmed by the disappearance of the signal at 3019-3030 cm^{-1} in IR spectra which is typical for hydroxyl group of azophenols and by the appearance of an intensive absorption band at 1260-1280 cm^{-1} which can be assigned to the antisymmetrical valence vibrations of the C-O-C group and a moderate absorption band due to the symmetrical valence vibrations of the C-O-C group at 1013-1014 cm-1 [1].

For the five chloro-azomonoethers, measurements were made to determine the decomposition kinetics in an air stream with a flow rate of 150 cm^3 min^{-1}, at heating rates of 2, 4, 6, 8 and 10 K min^{-1}. Kinetic calculations with the program TKS-SP 1.0 [2-3] to determine non-isothermal kinetic parameters of heterogeneous reactions allowed obtaining the activation energies of oxidative decomposition processes. The following figures show the thermoanalutical curves for the decomposition of the chloro-azomonoether in the figure, at the heating rate of 6 K min^{-1}, as well as the activation energy diagrams of the first decomposition step, at different degrees of conversion, for all compounds.





The five chloro-azomonoethers were also studied in terms of optical and spectral properties, quantum calculations of interactions with protein, optically and thermally induced cis-trans transitions in these azo compounds.

Acknowledgment „This work was supported by the grant POCU/993/6/13 -153178, co-financed by the European Social Fund within the Sectorial Operational Program Human Capital 2014 – 2020.

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Poster Presentation 2

The determination of the hydro-generator efficiency through the calorimetric method

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It is known that not always the functioning of a hydro- generator takes place in optimal conditions regarding the yield. The exploitation of a high power hydro- generator in low yield conditions can lead to high energy losses with the consequences streaming from this fact. The present paper proposes to present a simple determining method of the synchronous vertical hydro- generator yield by an indirect method, the calorimetric method for evaluating the losses of a hydro- generator.

The yield is determined by summing up the separate losses in several functioning regimes of hydro- generators, namely: unstressed empty functioning, stressed empty functioning and symmetric try phased short circuited functioning.

Thus, there is presented a method of determining the losses in stator iron, in the coil age of the stator and rotor and in the venting, respectively the supplementary losses by measuring the evacuated heat via the cooling agent, which is the air used by the motors on the rotor, air that takes up the losses from the generator and transmits them to the cooling agent-the water from the stator air coolers.

The temperature of the cooling agent, temperature of the stator air coil of the hydro-generator, the temperature of the cooling water, the temperature of the generator hood, all are measured with thermoresistance, while the air speed is measured with the anemometer.

By measuring the drop in temperature and the used air volume through the air coolers, one can observe sufficiently precise the proofs of the generator losses.

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Poster Presentation 3

Determining the stability of the power transformer insulation at high temperatures

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Due to the exposure during operation to higher than normal temperatures and to the presence of chemical compounds in the electro-insulating oil, the solid insulation of power transformers undergoes a process of forced degradation that ultimately determines the shortening of the operating life or the premature breakdown of the insulation [1-2]. The oxidation process is all the more intense as the transformer operates at a higher temperature, generating the diffusion process of water in the oil and in the solid insulation.Following this process, oil-soluble oxidizable products are formed, which are deposited on the transformer windings and form acidic reactions, blocking the cooling of the transformer. Since the insulation resistance is directly influenced by the temperature, varying inversely proportionally, the periodic measurements should be performed every time at the same temperature, which is impossible in exploitation[1-3]. For this reason, the measured values of the insulation resistance are recalculated at a reference temperature, usually 20ºC, respectively the reference temperature given by the manufacturer[2-3]. In this paper, the causes that generate the excessive heating of the insulation of power transformers in operation are highlighted and solutions are developed so that the dielectric losses are as small as possible and the operating time is as long as possible. To obtain the concrete results, the ANSYS thermal analysis application was used as a simulation method, as well as the real data obtained from the cases encountered in exploitation.

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Poster Presentation 4

Thermal behaviour of a coating based on epoxy resin and castor oil

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Epoxy resins are known as being one of the most versatile, low cost and high fabrication yield class of thermosetting polymers with excellent thermo–mechanical, electrical and physico–chemical properties. Epoxy resins are applied in many applications, ranging from adhesives to aerospace materials [1-4]. The final features of epoxies are determined by chemical structure and components from the mixture (plasticizers, hardeners, fillers, dyes, reactive diluents, etc.). This study describes the obtaining and characterization of a flexible epoxy resin from castor oil maleate and diglycidyl ether of bisphenol A (DGEBA). The structure was synthesized via esterification with maleic anhydride and characterized by FTIR and ^{1}H–NMR spectroscopy. Thermal degradation was assessed by TGA in nitrogen flow rate up to 600 ^{o}C. The global kinetic parameters were calculated with the aid of the Friedman isoconversional method. The kinetic results showed a three stage thermal decomposition mechanism, represented by diffusion, n^{th} order and Avrami–Erofeev reaction models. There were obtained the kinetic parameters values describing each stage of thermal decomposition through a multivariate non–linear regression method. TGA/DTA–FTIR–MS coupled methods were used in identifying the gaseous fragments evolved during thermal degradation.

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Poster Presentation 5

Pottery samples from the settlements and burial ground at Pecica – East site (Pecica, Arad County, Romania): analysis through hyphenated techniques

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The study presents the results from the analysis of pottery samples from the archaeological sites (Pecica East-Forgaci/Lucaş, Pecica-East/Duvenbeck) at Pecica-East (Pecica, Arad County, Romania). The sites are settlements and burial grounds in use during the Neolithic, the Copper Age (Aeneolithic to Bronze Age transition), as well as during the Medieval period [1-3].

The analyzed samples come from 12 pottery sherds, belonging to the Aeneolithic period (Tiszapolgár culture) and Copper Age (Bodrogkeresztúr culture). The samples cover the main types (fine, semifine, coarse and painted ware). The purpose of the analysis was to determinte the composition of the wares and firing temperatures.

The analysis was conducted using complementary techniques (TG/HF, FT-IR, XRD, SEM and XRF) [4-7].

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Poster Presentation 6

Polysaccharide membranes as a delivery agent for local anesthetic drugs

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The main objective of this study was to obtain polysaccharide membranes in which four different amide-type local anesthetic drugs were incorporated. Polysaccharides are known for their film-forming properties and are being extensively studied for food and non-food applications. These properties depend on the type of material used as the structural matrix (morphology, molecular weight, charge distribution), film manufacturing conditions (solvent, pH, concentration, temperature, etc.), type and additive concentration (plasticizer, cross-linking agent, antimicrobial agent, antioxidant, etc.) [1,2]. Local anesthetics block peripheral nerves and are used to prevent pain, provide painless surgical or dental procedures, control pain during labor or postoperative recovery, and manage chronic pain [3].

Two types of polysaccharide membranes were obtained (type A and type B membranes) in which different local anesthetic drugs were incorporated. Both types of membranes were obtained as thin film. Due to the different mass ratios between polysaccharides and plasticizer, membranes have different aspects. Type A membranes are similar to cellophane, while type B membranes are similar to parafilm.

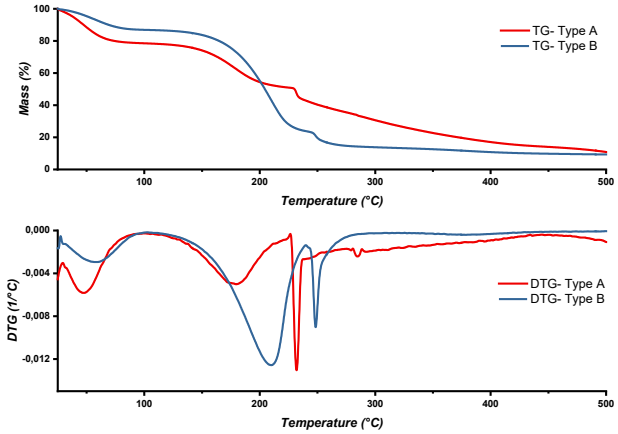

Figure 1. TG and DTG curves of control membranes.

As can be seen from Figure 1, even if the composition of the membranes differs, they show the same thermal decomposition processes. The only noticeable difference is the "intensity" of the second decomposition process that is more pronounced in the case of membrane B. This is due to the fact that this membrane is composed of two different polysaccharides, which present thermal processes in almost the same temperature limits, as type A membrane, but with a greater mass loss in the process corresponding to the thermal decomposition of the polysaccharide matrix.

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Poster Presentation 7

Pottery and clay samples from the Neo-Aeneolithic settlement Şoimuş - Avicola site/ Şoimuş - Teleghi (Șoimuș, Hunedoara County, Romania): analyzed using hyphenated techniques

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The purpose of this study is to present results from analyzing pottery samples from ceramics found within the archaeological site Neo-Aeneolithic settlement Şoimuş - Avicola / Şoimuş - Teleghi site (Șoimuș, Hunedoara County, Romania), a settlement inhabited during the Neolithic, Aeneolithic, Bronze Age, first Iron Age (Hallstatt) periods, as well as during the Roman era and Medieval times [1-3].

The analyzed samples come from 10 pottery sherds, belonging to the Neolithic period of the settlement's existence and attibuted to Vinča culture (phase A3 to phase B1). The samples cover the main types (fine, semifine, coarse). The analysis was aimed at determining the composition of the wares and firing temperatures. The pottery's relation to local clay sources was also investigated through analysis of 3 clay samples from the site.

The analysis was conducted using complementary techniques (TG/HF, FT-IR, XRD, SEM and XRF) [4-7].

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Poster Presentation 8

Study of thermally induced interactions between active substances from the sartans class and various excipients

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Medicines from the sartan class (Irbesartan, telmisartan, azilsartan and valsartan) are used to treat patients with hypertension (high blood pressure) and those with certain heart or kidney diseases. The drugs work by blocking the action of angiotensin II, a hormone that constricts blood vessels and causes blood pressure to rise.

In order to successfully design a new pharmaceutical form, one of the main considerations in the beginning stages of the process is represented by the compatibility anhydrous lactose (Friesland Foods Domo, Holland), talc (Luzenac Pharma, Italy), magnesium stearate (Fluka, Germany), colloidal silica (Aerosil 200 Evonik Degussa, Germany), polyvinylpyrrolidone K30 (BASF, Germany), starch (Grain Processing Corporation, USA), Manitol. The binary mixtures were prepared by trituration of equal masses of Sartans and each excipient in agate mortars for 5 min. The solid samples were then sieved and transferred in sealed vials and kept under ambient conditions until analyses were carried out. Thermal induces interaction for binary mixture between Sartans and excipients was studied using a TG/DTG/HF (see Fig. 1) and FTIR study.

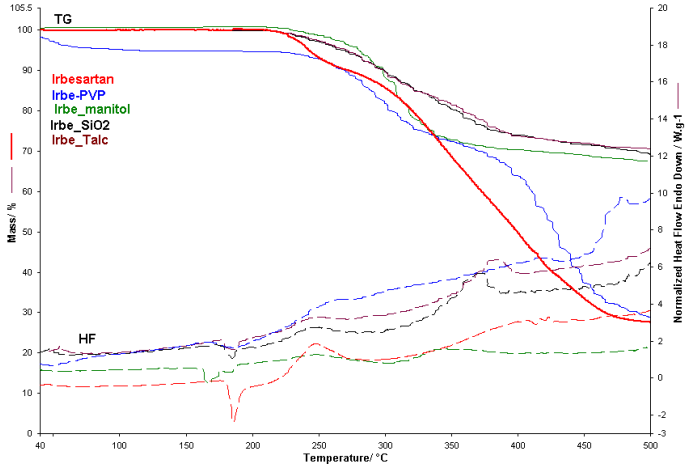

Fig.1. Comparative curves TG/HF for Irbesartan and binary mixture with PVP, Manitol, Talc, SiO_2

[1] V. Buda, B. Baul, M. Andor, D.E. Man, A. Ledeti, G. Vlase, T. Vlase, C. Danciu, P. Matusz, F. Peter, I. Ledeti. Solid State Stability and Kinetics of Degradation for Candesartan—Pure Compound and Pharmaceutical Formulation, *Pharmaceutics* 2020, 12, 86.

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Poster Presentation 9

Superionic Conductivity Modeling of NZSP NaSICON Synthesized by an Augmented SSR Method

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Less constrained by bandwidth limitations and sampling scarcity, broadband profiling in a wide temperature range, starting at the cryogenic threshold at -150 °C and extending to 200 °C, can be used to derive parameters of minimal variance for the Jonscher power law for ionic conductivity; these are employed to model the superionic regime over elevated temperatures and frequencies beyond the limits accessed by contemporary electrochemical impedance spectroscopy (EIS) equipment [1–3]. We apply this technique to non-stoichiometric NaSICON based on the canonical NZSP formula with 5% excess sodium, synthesized by an augmented solid-state reaction (SSR) method. We thoroughly analyze broadband conductivity, dielectric permittivity, and electric modulus data over the extended temperature range. Activation energy anomalies and scaling distortions inherent to the Arrhenius approximation are investigated, and an alternative formulation based on linearized difference equations is proposed to remedy these issues. With Cole-Cole analysis establishing non-Debye relaxation behavior, dissipation analysis is employed to identify relaxation bands, used for extracting initial condition parameters for the Jonscher power law. Finally, simulations of the AC dispersion region at high temperatures and frequencies suggest the dominance of polaron tunneling mechanisms instead of the classical ion hopping mechanism assumed for NaSICON, in line with the latest insights on superionic conduction.

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Poster Presentation 10

Synthesis and characterization of silver ion doped hydroxyapatite

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Hydroxyapatite (HA) is an important and one of the most studied biomaterials with a wide activity in the medical and also, dental fields, due to its biocompatibility and bioactivity. It is used in the construction of bone prostheses, pastes used to repair bone tissue or tooth enamel [1,2]. Doping this biomaterial with silver ions which present antibacterial properties, reduces the risk of hydroxyapatite contamination [3].

This paper presents a study on the synthesis and characterization of silver ion doped hydroxyapatite. The first step of this study was to establish the optimal parameters of the synthesis for hydroxyapatite, following the pH at which pure hydroxyapatite can be obtained using the chemical precipitation as a method. To synthesize hydroxyapatite, basic pHs as 8,00, 9,00, 10,00 and 11,00 were chosen, avoiding the precipitation of other phosphates.

After the optimal synthesis pH was established, silver ion doped hydroxyapatite was synthesized at different mass concentrations of 2%, 4%, 6%, 8% and 10%, respectively, using the steps chosen for the first method.

Following these two synthesis accomplished at different pHs and by doping with silver ions, the samples obtained were analyzed using Fourier transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD) (Fig.1), and also thermogravimetric analysis (TGA).

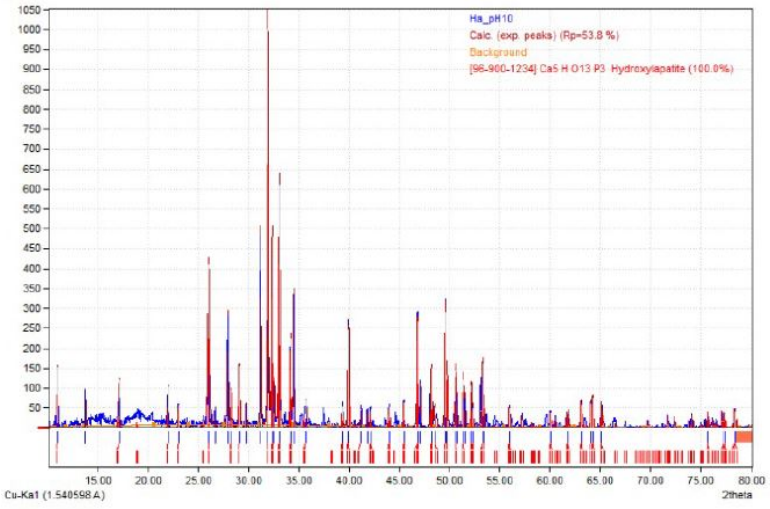

Fig.1. XRD spectra of calcinated HA-Ag 10% sample

[1] Y. Oshida, ”Hydroxyapatite: Synthesis and Applications”, Momentum Press, New York, 426

[2] V.S. Gshalaev, A.C. Demirchan, ”Hydroxyapatite: Synthesis, properties and applications”, Nova Biomedical, New York, (2013) 493

[3] Q. Yuan, A. Xu, Z. Zhang, Z. Chen, L. Wan, X. Shi, S. Lin, Z. Yuan, L Deng, ”Bioactive silver doped hydroxyapatite composite coatings on metal substrates: Synthesis and characterization”, Mater. Chem. Phys., (2018) 218: 130-139.

Poster Presentation 11

The properties variation of hydroxyapatite dispersed into polymer matrix during thermal treatment

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A simple process for the synthesis of ented[1]. Wet chemical method is a popular method to synthesize HAP and the use of organic macromolecules containing polar functional groups, such as COOH and OH can influence the synthesis of HAP because these ionizable side groups provide a greater affinity to positive Ca^{2+} ions and the nucleation of HAP crystals in the solution[2], [3].

CMC was used at different concentration (0, 0.25, 0.5, 0.75, 1.0 w/v) as an infiltration medium during the synthesis of HAP from calcium nitrate and phosphoric acid as sources of calcium and phosphorus, maintaining the concentration of the solution in order to have a Ca/P ratio at 1.67 and at a pH of 10.

It is expected that CMC will interact with precursors to direct the action and growth of hydroxyapatite, so that bioactivity occurs. The effect of the CMC content on the mineralization efficiency is monitored, in terms of the size, structure and morphology of the nanocomposite materials obtained. The effects that CMC has on these properties were monitored by means of SEM, FT-IR, EDX and TGA during the thermal treatment and at the end it in order to see how the system evolves till crystallisation of HAP occurs.

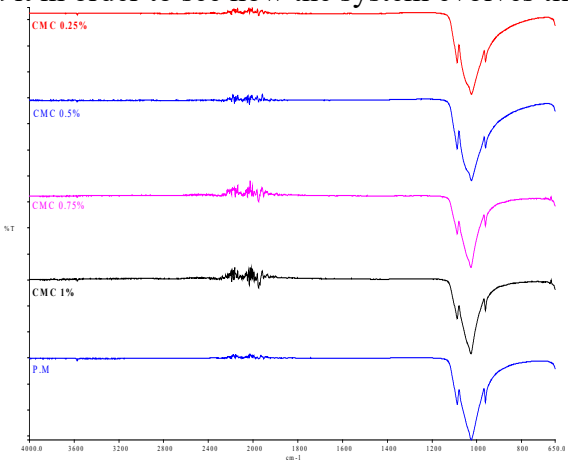
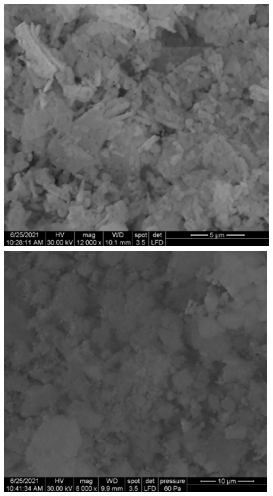


Fig. 1. Spectra of calcinated samples at 900 ˚C



(a)

(b)

Fig. 2. SEM of calcinated CMC 0.25 (a) and 1 (b)

[1] M. Sayed, H. F. El-Maghraby, F. Bondioli, and S. M. Naga, *J. Appl. Pharm. Sci.*, vol. 8, no. 3, 023–030, 2018.

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Poster Presentation 12

Coagulant – antibiotic scaffold systems for dental application

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The present investigation aimed to formulate and evaluate a new scaffold system based on coagulant-antibiotic for dental application. Various scaffold systems, including injectable[1] or polymeric[2] scaffolds, are available on the market for bone tissue, dental, oral, and craniofacial regeneration[3]. The formulated scaffold systems are based on Sodium Alginate (Alg): Vitamin K (K): cephalosporin (Cephalexin (Cep)/ Cefazolin (Cef)).

Cephalosporins are beta-lactam antimicrobials acting on the penicillin-binding proteins (PBPs), preventing them from closing vulnerable ends on dividing bacteria[4].

Before the scaffold system preparation, a compatibility study was performed between each component. Active substances, mixtures between individual components (Cep; Cef; Alg, K), and scaffold systems were analyzed using FTIR-UATR and thermogravimetry (TGA). See Fig. 1a, 1b for FTIR-UATR analysis of Cef; Cep.

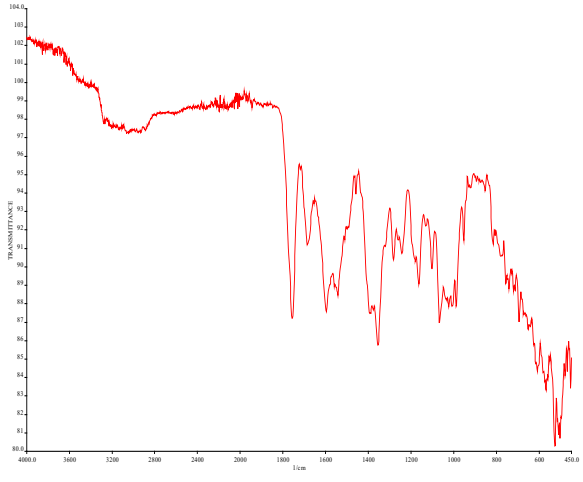

Fig.1a: FTIR spectra for Cef

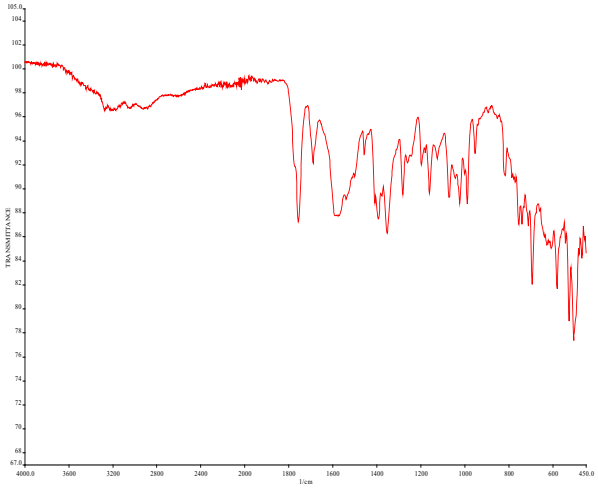

Fig.1b: FTIR spectra for Cep

[1] B. Chang, N. Ahuja, C. Ma, X. Liu, "Injectable scaffolds: Preparation and application in dental and craniofacial regeneration", Mater Sci Eng R, 111 (2017) 1-26;

[2] D.T. Wu, J.G. Mungaia-Lopez, Y.W. Cho, X, Ma, V. Song, Z. Zhu, "Polymeric scaffolds for dental, oral, and craniofacial regenerative medicine", Molecules, 26 (2021) 7043;

[3] A. Farzin, N. Bahrami, A. Mohamadnia, S. Mousavi, M. Gholami, J. Ai, "Scaffolds in Dental Tissue Engineering: A Review", Arch Neurosci, 7 (2019) 1-5;

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Poster Presentation 13

Composites with antibiotics, bisphosphonate and hydroxyapatite for dental applications

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Bone-grafting procedures have been used to regenerate bone within osseous defects, including that of the alveolar bone. The aim of the present study was to formulate new variants of synthetic and animal bone materials coated with different biopolymers, containing antibiotics (ampicillin and oxacillin) and drugs alendronate. These materials should act as a transmucosal drug delivery system alongside the bone base. Drug delivery systems, such as those based on polymers, can be designed to enhance the pharmacological and therapeutic properties of topically administered drugs.

To avoid drug-related complications, natural polymers such as chitosan, alginate, and kappa-carrageenan have been shown to be optimal materials for drug delivery due to their intrinsic biocompatibility. The aim of the synthesized materials is to incorporate active substances into biopolymers and use these to coat bone materials in granulated form.

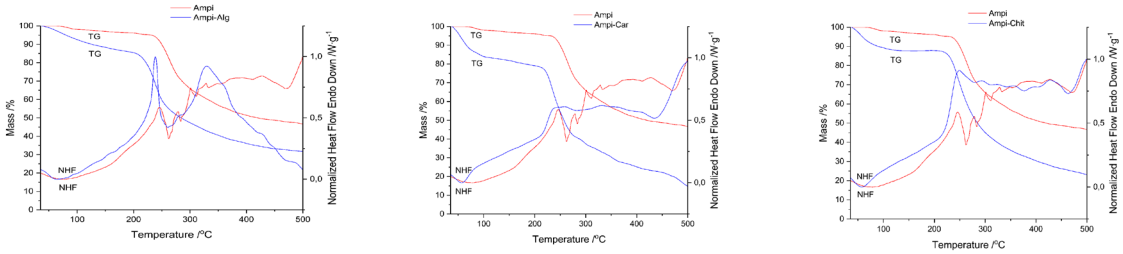

Fig. 1. TG/DTG curves for Ampi and binary mixture with biopolimers (example)

The binary, ternary and quaternary mixtures prepared between the components are analyzed by FT-IR spectroscopy, UV-Vis analysis, thermogravimetry (TG) (Fig.1) and scanning electron microscopy (SEM). The analyzes led to the validation of materials suitable for the controlled release of active substances, which have the greatest chance of increasing the speed of bone regeneration as well as supporting the local delivery of antibiotics, which currently requires administration in the form of tablets or injectables. These materials could be used to administer a smaller amount of antibiotics or alendronate avoiding the side effects experienced by some patients.

Poster Presentation 14

Kinetics of thermal degradation of pharma grade sulfobutylether sodium betacyclodextrin

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In this study, we set our goal in evaluating the solid-state stability and the decomposition mechanism of pharmaceutical grade sulfobutylether betacyclodextrin sodium (commercial name DexolveTM, manufactured and supplied by Cyclolab Ltd., Hungary, as a „generic" Captisol cyclodextrin), that was offered as gift sample from the producer. This pharmaceutical grade cyclodextrin excipient, produced and sold under DexolveTM is commonly used as a solubility and stability enhancer that acts in this manner by inclusion complex formation [1]. Up to the date, pharmaceutical grade sulfobutylether betacyclodextrin sodium (SBECD) is used in the formulation of several commercial products, but as well is studied for novel products, that are under development [1,2].

Since no references were found regarding comparative oxidative thermolysis and degradation kinetics of sulfobutylether betacyclodextrin sodium (SBECD) in comparison to betacyclodextrin (BCD), we aimed towards carrying these investigations according to some previous studies [3,4]. The kinetic protocol consisted in recording for each sample five thermoanalytical curves (TG/DTG/HF) in dynamic air atmosphere, at five different heating rates β = 5, 7, 10, 12 and 15 °C/min, followed by the data processing using ASTM E698 kinetic method as preliminary one, then the employment of isoconversional methods of Flynn-Wall-Ozawa (integral method) and Friedman (differential method) and later, the modified non-parametric kinetic method (NPK). Solely the NPK method allowed a concrete separation of individual physical/chemical processes involved in degradation of investigated compounds. Also, an in-mirror discussion was carried out for the effect of inserting sulfobutyl moiety on BCD skeleton over its thermal stability.

Acknowledgements: This work was supported by the PN-III-P1-1.1-TE-2016-1165 project (RECOTHER).

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Poster Presentation 15

Instrumental investigations of telmisartan-aminoacids binary adducts

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Telmisartan (TELM, Figure 1) is an active pharmaceutical ingredient used in the treatment of hypertension, heart failure, and diabetic kidney disease, being a reasonable initial treatment for high blood pressure [1].

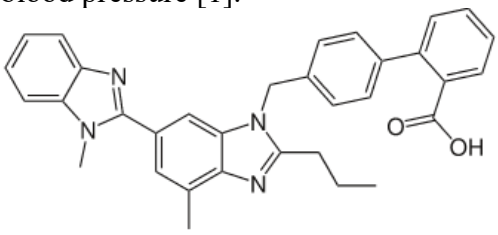

Figure 1. Chemical structure of TELM

TELM is also the first angiotensin receptor blocker to show a promising role in reducing cardiovascular risk [2]. Similar to other sartans, TELM belongs to BCS class II drug with low solubility at physiological pH [3], so methods for improving its solubility are investigated.

The formation of binary adducts such as cocrystals and salts usually determines the increasing of stability and solubility of pharmaceuticals, so in this paper we focused into development of several adducts of TELM with the following aminoacids: L-aspartic acid, DL-tryptophan, L-alanine, L-leucine, L-valine, L-cysteine, L-cystine and L-glycine and their investigation by ATR-FTIR spectroscopy and thermal analysis (TG/DTG/HF).

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Poster Presentation 16

Heptakis(2,6-di-O-methyl)-β-cyclodextrin inclusion complex of olmesartan medoxomil. Compatibility with excipients

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Olmesartan medoxomil, an ester-type prodrug (OLM, Figure 1) is a non-peptide antagonist which selectively and competitively inhibits the type-1 angiotensin II receptor, being used in the treatment of hypertension [1,2]. Belonging to the class II drug in the Biopharmaceutics Classification System (BCS), OLM exhibits very low aqueous solubility and the improvement of its biopharmaceutical profile can be realised by the increase of its solubility in the presence of cyclodextrins [3,4].

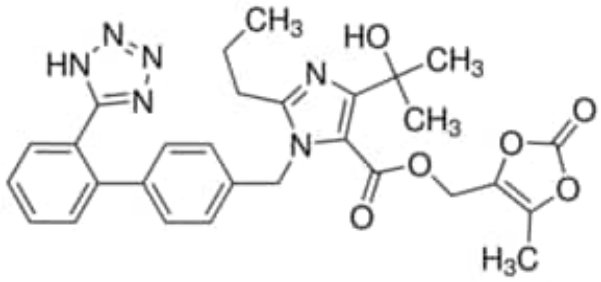

Figure 1. Structural formula of OLM

In this study, the compatibility between OLM inclusion complex with heptakis(2,6-di-O-methyl)-β-cyclodextrin (DIMEB) and starch, lactose, magnesium stearate and talc was studied by means of thermoanalytical tools (TG/DTG/HF), powder X-ray diffractometry (PXRD) and universal attenuated total reflectance Fourier transform IR spectroscopy (UATR-FTIR). The complementarity of the investigational methods is discussed, along with the existence of interactions between the components of the analysed systems.

[1] Warner GT, Jarvis B. Olmesartan medoxomil. Drugs. (2002) 62(9) 1345-53
[2] Brunner HR. J Hum Hypertens. (2002) Suppl 2:S13-6.
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Poster Presentation 17

Transmucosal absorption of antibiotic-anesthetic polymer-based systems for dental use

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Polymeric membranes are frequently used for bone regeneration in oral and periodontal surgery. Polymers provide adequate mechanical properties to support oral function and also poses some porosity with interconnectivity to permit for cell proliferation and migration [1].

These occlusive membranes must fulfill several criteria, including space maintaining capacity, mechanical properties, osteoconductivity/osteoinductivity, and biocompatibility [2]. Currently, it seems that natural and artificial polymers are the best candidate materials to comply with most of these prerequisites [3].

The purpose of this study is represented by obtaining and characterizing alginate-based membranes in which antibiotics and local anesthetics were incorporated as active principles. Amoxiklav was used from the class of antibiotics (fig.1), and local anesthetics from the class of amides (articaine, mepivacaine, bupivacaine, ropivacaine) were used as anesthetics. The analysis methods used in this study were FTIR-UATR spectroscopy, thermogravimetric analysis and SEM.

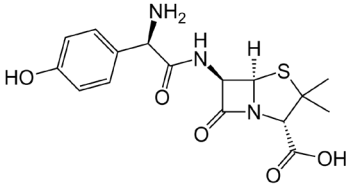

Fig. 1. Chemical structure of Amoxiklav (Amoxicillin/clavulanic acid)

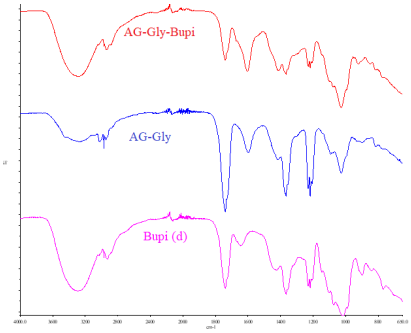

Fig. 2 IR Spectrum of AG-Gly-Bupi patches, AG-Gly patche and Bupi dissolved

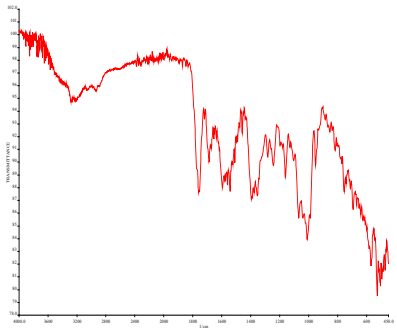

Fig. 3 IR Spectrum of Amoxiklav

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Poster Presentation 18

Theoretical and instrumental approach for the development of co-crystals with mirtazapine and opipramol

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For active pharmaceutical ingredients (API) with poor water solubility, such as the atypical antidepressants mirtazapine (MRT) and opipramol (OPI), the preparation of effective drug formulations can be challenging. Numerous options are currently available to overcome this inconvenience, the use of co-formers among them. Amino acids have been evaluated for the formation of co-crystals, literature showing an increase in the solubility, bioavailability and stability of the API when associated with these [1].

The study began with a molecular modelling evaluation meant to assess the co-crystal possibility formation between the APIs and the amino acids selected as co-formers. The solid-state samples were prepared in a 1:1 molar rate between MRT or OPI as APIs and each amino acid, namely glycine, alanine, glutamic acid and aspartic acid. As instrumental techniques, ATR-FTIR spectroscopy (4000-400 cm^{-1} spectral range), thermal analysis (synthetic air atmosphere, β = 10 °C·min^{-1}) and powder X-ray diffractometry (PXRD) were used.

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[1] I. Nugrahani, M.A. Jessica, Molecules, 26 (2021) 3279