FACULTY OF INDUSTRIAL CHEMISTRY AND ENVIRONMENTAL ENGINEERING



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RESEARCH CENTRE PROTECTION AND DEPOLLUTION WATER ENGINEERING AND ENVIRONMENTAL ANALYSIS OF INDUSTRIAL PROCESS - P.D.W.E.E.A.I.P.

GENERAL PRESENTATION

This research centre is a CNCSIS accredited, type C, research centre reapproved by CNCSIS in 12.09.2006, according to CNCSIS certificate nr. 28. The director of the Center is **Prof. dr. eng. Petru Negrea**.

MAIN ACTIVITIES

The Centre accomplishes research and design in the following topics:

- Environmental analysis of industrial processes
- Drinking and industrial water treatment
- Wastewater treatment
- Process control equipments for research plants in chemical industry
- Control systems using computers for researching plants and low tonnage plants in chemical industry
- Intensive methods for the exoneration of soil from radioactive minerals exploitation and processing areas in the condition of natural disasters or entropic accidents
- Mathematical modeling and numerical simulation of environmental pollution and depollution processes
- Modeling, simulation and process control
- Heat transfer organic agents
- Unit processes
- Magnetic Fluids: Preparation, Characterization and Applications
- > The Intensification of Transfer Processes
- Rheological characterization of the substances
- Studies and projects for thermo-technical installations of the silicates industry
- Electrochemical processes
- Obtaining and characterization of oxide compounds

CONTACT

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RESEARCH FIELDS

Environmental analysis of industrial processes

Keywords: environmental, pollution, waste

> Drinking and industrial water treatment

Keywords: water treatment, drinking water, industrial water

Wastewater Treatment

Keywords: waste water treatment, pollution

Process control equipments for research plants in chemical industry

Keywords: measuring, control devices

Control systems using computers for researching plants and low tonnage plants in chemical industry

Keywords: process control, research and low tonnage plants

Intensive methods for the exoneration of soil from radioactive minerals exploitation and processing areas in the condition of natural disasters or entropic accidents

Keywords: Climate changes, pollution, risk, sustainable chemistry, modeling

Mathematical modeling and numerical simulation of environmental pollution and depollution processes

Keywords: modeling, simulation, environmental protection

Modeling, simulation and process control

Keywords: modeling, simulation, optimization, process control, absorption-desorption with chemical reaction

Oily compounds extraction from waste waters using magnetic fluids

Keywords: extraction, magnetic fluid

> Coordinative compounds with organic ligands

Keywords: coordinative compounds, heterocyclic compounds, hydroxycarboxylic acids, pharmaceutical substances, pigments, dyes

Synthesis of nanocomposites with controlled magnetic, optic and catalytic properties

Keywords: nanoparticles, sol-gel, silica, magnetic, catalytic, polyols

Homo-and heteropolynuclear compounds with organic ligands

Keywords: organic ligand, polinuclear compound, magnetic materials, catalysts, pigments, ferrites, chromites

Physical Chemistry. Chemically Active Species Grafted on Polymer-Supports

Keywords: catalysis, homogeneous catalysts, heterogeneous catalysts, polymer-grafted catalysts, polymer-grafted reagents, polymer-support

Physical Chemistry. The obtaining and characterization of some oxide compounds

Keywords: solid-state, oxide compounds, unconventional methods

Organic Electrochemistry

Keywords: organic electro synthesis, organic electro reduction and oxidation

Electro catalysis

Keywords: skeleton electrodes, thermal arc spraying, potentiometer sensors

Electroplating

Keywords: copper, zinc, nickel electrodepositing, brighteners

> Fuel Cells

Keywords: fuel cells, skeleton electrodes, proton exchanges membrane, anion exchange membrane

Synthesis of ceramic materials through hydrosilicatic forerunners

Keywords: ceramic, hydrosilicatic, synthesis

Semi conducting glasses. Fast ion-conducting glasses. Redox equilibrium in glasses. Low melting glasses for fusion type application

Keywords: conducting, glasses, redox equilibrium, vitreous systems

Ceramic glazes. Synthesis and characterization of thermo resistant pigments

Keywords: ceramic glazes, thermo resistant pigments, synthesis method

Chemistry and technology of building materials

Keywords: cements, mineral binders

Mathematical modeling and numerical simulation of soil depollution processes.

Researches in WATER TREATMENT AND PURIFICATION

The activity intensifying and diversifying of the industrial processes leads to the quality degradation of water sources, with important implications for water supplies. In this context it is important to research and to elaborate some treatment and purification technologies, more efficient and at low costs. The research activity was concerning with the majority of aspects involved by water chemistry and technology, as follows:

- physical and chemical characterization of water supplies and of wastewaters
- researches concerning water treatment for drinking and industrial purposes
- researches concerning the technologies of industrial and municipal wastewater treatment

Results of the research activity were published in journals of specialty and communicated at the national and international Symposia.

RESEARCH TEAM

Georgeta Burtica, Aurel Iovi, Petru Negrea, Rodica Pode, Ioan Ursoiu, Adina Negrea, Eugen Lungu, Marius Gheju, Florica Manea, Laura Cocheci, Giannin Moșoarcă, Lavinia Lupa, Mihaela Ciopec.

Researches in INORGANIC CHEMICAL TECHNOLOGY

Different processes for obtaining of the new products, with superior qualities have been studied (chemical fertilizers with microelements, inorganic salts, etc.), for turning to good account of the native raw materials, industrial wastes and for the recovery of the useful compounds from wastewaters.

Researches in:

- mineral fertilizers: urea, ammonium nitrite, NP, NPK, fertilizers with microelements
- improving and modernizing of the technological processes
- Turning to good account of some native minerals zeolites for wastewaters treatment and for the obtaining and conditioning of the fertilizers with microelements.

The results of researches were applied in industry.

RESEARCH TEAM

Petru Negrea, Georgeta Burtică, Rodica Pode, Laura Cocheci, Lavinia Lupa, Mihaela Ciopec

Researches in PROCESS CONTROL EQUIPMENTS FOR RESEARCH PLANTS IN CHEMICAL INDUSTRY

Some specific control equipments for research plants from chemical industry (measurement and control of small and micro gas and liquid flows, gas and liquid compositions, pressure) using as information support low pressure signals (500-3000 N/m²).

Elaboration, design and realization of a high performance reference models.

Keywords: measuring, control devices

RESEARCH TEAM

Marcel Suta, Carmen Rusnac, Alina Brusturean

Researches in CONTROL SYSTEMS USING COMPUTERS FOR RESEARCHING PLANTS AND LOW TONNAGE PLANTS IN CHEMICAL INDUSTRY

Realization of some specific control equipments using computers and process interfaces for automation of laboratory, research and low tonnage plants from chemical industry.

Elaboration, projecting and realization of control equipments using computers, process interfaces and proper software programs.

RESEARCH TEAM

Marcel Suta, Carmen Rusnac, Alina Brusturean

Researches in INTENSIVE METHODS FOR THE EXONERATION OF SOIL FROM RADIOACTIVE MINERALS EXPLOITATION AND PROCESSING AREAS IN THE CONDITION OF NATURAL DISASTERS OR ENTROPIC ACCIDENTS

Chemical decontamination of soil in the presence of ultra-sounds

Mathematical models and methods regarding the transfer mechanism in solid-liquid heterogeneous systems for the selection of optimal hydrodynamic parameters

Implementation of interface equipment in measurement devices

Keywords: Climate changes, pollution, risk, sustainable chemistry, modeling

RESEARCH TEAM

Carmen Rusnac, Gabriela Alina Brusturean, Dana Silaghi – Perju

Researches in MATHEMATICAL MODELING AND NUMERICAL SIMULATION OF ENVIRONMENTAL POLLUTION AND DEPOLLUTION PROCESSES

Mathematical modeling and numerical simulation of soil depollution processes

Elaboration of analytical and statistical models of air pollution phenomenon

Waste recycling process control and optimization

Keywords: modeling, simulation, environmental protection

RESEARCH TEAM

Carmen Rusnac, Gabriela Alina Brusturean, Dana Silaghi Perju.

Researches in MODELING, SIMULATION AND PROCESS CONTROL

Modeling and simulation of chemical processes using programming languages and software in process engineering: MATLAB, HYSIS, Aspen Plus, Aspen Custom Modeler;

Apply chemical reactor analysis, process modeling, simulation and optimization to chemical and petrochemical plants and find out solutions for industrial problems;

Modeling, simulation and process control of absorptiondesorption with chemical reaction processes.

RESEARCH TEAM

Teodor Todinca, Carmen Rusnac, Alina Brusturean

Researches in OILY COMPOUNDS EXTRACTION FROM WASTE WATERS USING MAGNETIC FLUIDS

It was studied the oily fraction recovery (especially oil products) from waste waters using magnetic fluids. The process is strongly influenced by the magnetic field presence; both the oily fraction and the magnetic phase could be recovered;

RESEARCH TEAM

Andra Tamas.

Researches in THE PERFORMANCE OF THE COLUMNS WITH STRUCTURED PACKINGS

The structured packing present a high efficiency by comparison with the random packing because of the very high specific surfaces. It was followed the knowledge of wettability degree influence in extraction or rectification processes. The aim of the future experiments is the increase of wettability degree through electrochemical or chemical activation

RESEARCH TEAM

Andra Tamas

Researches in CONDITIONING MODELS OF SEWAGE SLUDGE

The aim of this research consists in efficiency evaluation of chemical conditioning models by calculation of the sludge volume index (SVI), the specific resistance to filtration to improve sludge dewatering, as well as appropriation of a statistic mathematic model for the correlation of the obtained results.

RESEARCH TEAM

Vasile Pode, Andra Tamas

Researches in NANOCOMPOSITES WITH CONTROLLED MAGNETIC, OPTIC AND CATALYTIC PROPERTIES

Nanocomposites of type ferrite and ferrite/SiO₂ were synthesized trough two original methods: the thermal decomposition of some heteropolynuclear complex compound (with hydroxocarboxilic anions as ligands) and a modified sol-gel methods.

The fine nature of the obtained nanoparticles gives to the synthesized nanocomposites special magnetic properties that can be used in potential applications. Studies have been made in order to establish the dependence between the synthesis conditions, the dimensions of nanoparticles and their properties.

Studies have been made for the synthesis of hybrid polyol-silica matrix, correlation between synthesis conditions and textural properties of the silica matrix, for its use as support for some catalysts.

Studies are going to be made for the synthesis of metallic nanoparticles in silica matrix, with special properties and for the use of these materials as thin films for biological and environmental applications.

RESEARCH TEAM

Mircea Ștefănescu, Marcela Stoia

Researches in HOMO - AND HETEROPOLYNUCLEAR COMPOUNDS WITH ORGANIC LIGANDS

Synthesis and characterization of some inorganic compounds in order to obtain simple and mixed oxides with catalytic, pigmental and magnetic properties

A new synthesis method has been carried out in order to obtain some homo - and heteropolynuclear compounds with hydroxocarboxylic acid anions as ligands. The simple and mixed oxides with special properties have been obtained by thermal conversion of some complex compounds

RESEARCH TEAM

Mircea Niculescu, Mircea Ștefănescu, Marcela Stoia, Raluca Dumitru, Ilie Julean

Researches in PHYSICAL CHEMISTRY OF SOLIDS. OBTAINING AND CHARACTERISATION OF SOME OXIDE COMPOUNDS

The properties of the oxide compounds formed by reactions in the solid state are significantly dependent on the synthesis method used, respectively on the initial state of the reactants.

For the obtaining of some oxide compounds, different synthesis methods have been used: a) the sol-gel method; b) thermal conversion of certain

complex combinations; c) combustion synthesis; d) hydroxide co precipitation; e) annealing of salts and/or oxides mixtures. The reactivity of the systems was studied comparatively for the different synthesis methods used.

RESEARCH TEAM

Cornelia Păcurariu, Dumitru Becherescu, Ioan Lazău, Radu Ioan Lazau, Robert Ianos, Marius Jurca

Researches in ORGANIC ELECTROCHEMISTRY

Electrochemistry represents today a very convenient method for the synthesis of a variety of important organic compounds, which in many cases have been extended to an industrial scale.

Since 1982 theoretical and practical investigations have been made upon electrode processes of organic electrochemistry. The synthesis of quinine, hydroquinone, and ethylene glycol has been analyzed, especially in undivided electrochemical reactors. Studies upon mediated reduction and oxidation of organic compounds have been undertaken.

RESEARCH TEAM

Nicolae Vaszilcsin, Andrea Kellenberger, Mircea Dan, Narcis Duțeanu

Researches in *ELECTROCATALYSIS*

Obtaining, characterization and application of the electrodes with catalytic activity.

Methods for the preparation of electrocatalytic films have been elaborated in our research team, based on the thermal decomposition of some complex compounds and through thermal arc spraying technique. These films have been characterized through scanning electron microscopy, X-ray diffraction and voltammetry. The practical applications refer to water electrolysis and to the synthesis of some organic compounds.

RESEARCH TEAM

Nicolae Vaszilcsin, Andrea Kellenberger, Mircea Dan, Narcis Duțeanu

Researches in *ELECTROPLATING*

Obtaining and characterization of metal coatings

Studies regarding the influence of the nature of the galvanic additives upon the quality of the metal deposition have been made. Metal layers have been characterized by X-Ray diffraction, scanning electron microscopy and energy dispersive X-ray microanalysis. The practical applications refer to the replacement of the cyanide galvanic baths with non-toxic ones.

RESEARCH TEAM

Nicolae Vaszilcsin, Andrea Kellenberger, Mircea Dan, Narcis Duțeanu, Radu Bănică

Researches in FUEL CELLS

The conventional energy systems are the main source of pollution on our planet. Considering the decreasing of the Earth's resources of hydrocarbons, it is necessary to improve an alternative energy conversion technology such as the fuel cells. This technology offers many attractive possibilities for reducing the air pollution, diminishing climate changes and preserving our natural resources. Widespread application of this technology is still prohibitive because materials used to made electrodes are expensive.

The aim of our research is the reducing of the H_2 - O_2 fuel cell costs by changing the Pt based electrodes with non-noble based electrode obtained using various methods (thermal decomposition, thermal spraying).

RESEARCH TEAM

Nicolae Vaszilcsin, Andrea Kellenberger, Mircea Dan, Narcis Duțeanu, Radu Bănică

Researches in SYNTHESIS OF CERAMIC MATERIALS THROUGH HYDROSILICATE FORERUNNERS

The use of hydrosilicatic forerunners from precipitate reactions to obtain at lower temperatures some high quality ceramic materials such as: wollastonite, enstatite, diopside, willemite, anortite, magnesium spinel and a multitude of oxidic pigments.

The studies in this field have been made at the "Politehnica" University of Timişoara since 1985. The researches have been materialized in a laboratory synthesis method of the materials involved. Verification of the behavior of some synthesized materials in industrial circumstances.

RESEARCH TEAM

Ioan Lazău, Dumitru Becherescu, Marius Jurca, Radu Ioan Lazău

Researches in SEMICONDUCTING GLASSES. FAST ION CONDUCTING GLASSES. REDOX EQUILIBRIA IN GLASSES. LOW MELTING GLASSES FOR FUSION TYPE APPLICATION

Studies regarding electrical conductivity in new molybdenum glass systems. Influence of different transitional ions upon conduction properties of glasses was studied. Synthesis and characterization of fast ion conducting glasses containing Ag^+ , Li^+ and Cu^+ ions. Glasses with optimal ion conductivity were design. New fast ion conducting glasses were obtained. The behavior of redox equilibrium Mn^{2+}/Mn^{3+} was studied in the following binary systems: SiO₂-R₂O, P₂O₅-R₂O and B₂O₃-R₂O.

The influence of melting conditions (reducingoxidizing) upon the presence of Ti^{4+} was studied, as well as its relationship with the iron present. The reciprocal influence of Ti⁴⁺ and other different ions usually present as impurities upon the color in industrial glasses was studied.

Design, synthesis and characterization of low melting glasses for fusion type applications was studied. The reciprocal influence fusion glass-support glass was investigated using microscopic techniques.

RESEARCH TEAM

Adina Lația, Cosmin Vancea

Researches in CERAMIC GLAZES. SYNTHESIS AND CHARACTERIZATION OF THERMORESISTANT PIGMENTS

The research field extends over the conventional and unconventional synthesis methods for thermoresistant pigments designed to the ceramic industry (ceramic glazes and enamels), characterization of the obtained pigments from the point of view of crystallochemical structure and color. At the same time, the behavior of the synthesized pigments in the glass generating melt is being pursued.

RESEARCH TEAM

Ioan Lazau, Cornelia Păcurariu, Dumitru Becherescu, Radu Ioan Lazau, Robert Ianos

Researches in CHEMISTRY AND TECHNOLOGY OF BUILDING MATERIALS

Local waste materials are analyzed in order to use their potential resources in the field of building materials. Ecological and economical implications of waste or natural deposits especially form Romanian's regions: Transylvania and Banat, containing minerals with possible interest for buildings materials products and technology are investigated.

RESEARCH TEAM

Aurel Ștefan Todinca

RESEARCH PROJECTS

1. PN II ZEO-NANOSPP-56/2009: Synthesis of functionalized zeolite materials with doped titanium dioxide nanoparticules and testing in water potabilization pilot stations

Value:	0,000 LEI
Director:	Prof.dr.eng. Georgeta BURTICĂ
Members:	Asist. Prof. dr. eng. Florica MANEA
	Eng. Cristina PROCA
	Eng. Rodica NEAGU

FIELD DESCRIPTION

Studies over the doped TiO2 nanocrystals getting through alternative methods, processing to the efficient solutions to get the modified zeolitic materials with TiO2 nanocrystals doped with metallic/nonmetallic ions, like the characteristics of source and drinking water and dinking water decontamination

ACTIVITIES AND RESULTS

Studies of concordance on the TIO_2 nano crystals doped with metallic/non-metallic ions trough RX diffraction, Electronic microscopy (TEM, AFM, SEM) - UV-VIS spectrometry. Preliminary researches of synthesis of zeolitic materials functionalised with TiO₂ doped with non-metallic ions. Semination of the results on large scale, trough national and international communication and publishing.

2. **IDEI - 927/2009**: Integrated concept about depollution of waters with arsenic content, through adsorption on oxides materials, followed by immobilization of the resulted waste in crystalline matrices

Value:105.830 LEIDirector:Lect.dr.eng. Adina NEGREAMembers:Prof. dr. eng. Ioan LAZAUAssist. Dr. eng. Lavinia LUPALect.dr. eng. Radu LAZAUC.S. dr. eng. Mihaela CIOPECPhD student eng. Suba Mariana

FIELD DESCRIPTION

The project is connected to a main direction of the international researches, main field environment sustainable development - global changing and brings fundamental elements in constitution of capable research teams for the competitions in european programs. As part of this project the depollution of waters with arsenic content is intended, through adsorption on synthetic oxides materials. As adsorbent materials sludge with iron oxides content resulted from other processes will also be studied. The absolute novelty of this project consists in using the waste resulted after arsenic adsorption as auxiliary raw material in glasses manufacturing; this procedure assures not only the pollutant immobilisation in the crystalline matrix, but even the substitution of a classical raw material As₂O₃ and the concomitant capitalization of the components resulted from adsorbent - in full agreement with the principles of the sustainable development.

ACTIVITIES AND RESULTS

The synthesis and characterisation of the oxide materials used as adsorbents (obtaining, chemical analysis, specific surface area, adsorption capacity, adsorption degree). There will be synthesized in laboratory a series of oxide materials based on iron or on silicates, which will be characterised together with the unconventional ones. Are anticipated new posibilities of the oxide composition and adsorbent structure optimisation, so that this can be used as auxiliar raw material in crystalline matrix obtaining. Testing – experimental determination of adsorption, as well as kinetic study.

3. **PN II- 72-171/2009**, *Micro porous sensors with polianiline functionalised with pendant groups, innovative materials used in the identification and control of the Parkinson disease.*

Value:	0,000 LEI
Director:	Assoc.prof.Ph.eng.Andrea KELLENBERGER
Members:	Prof. Ph. eng. Nicolae VASZILCSIN
	Assist. Phd eng. Mircea Laurentiu DAN
	Assist. Ph. eng. Narcis DUTEANU
	Phd eng. Radu BANICA
	Student Anuta NASUI
	Student Raluca NITOI
	Student Diana MIHART

FIELD DESCRIPTION

Electrochemical sensors based on polyaniline for the detection of dopamine in the Parkinson disease.

ACTIVITIES AND RESULTS

Reference materials study regarding the obtaining of the micro porous sensors with polinainlin functionalised with pendant groups.

4. **PN II- STEDIWAT- 32-125/2009**: Technicaldecisional support system for sustainable management of water.

Value: 24.636 LEI Director: Lecturer Ph eng. Florica MANEA Members: Prof. Ph. eng. Georgeta BURTICA Phd eng. Aniela POP Phd eng. Cristina PROCA Phd eng. Adriana BEBESELEA

FIELD DESCRIPTION

The development of some innovative technical support instruments, for monitoring, design and prediction which to be used for sustainable and incorporated management, at hydrographic basin level. Also, the development of the capacity of the collaboration, knowledge and communication transfer between universities and local / regional authorities of water resources management, users and other interest parts in the four studied basins (Prut,, Banat, Arges-Vedea, Olt) with impact on the sustainable development at the local and regional level.

ACTIVITIES AND RESULTS

Research base witch contain studies about: evaluation of the infrastructure and of the institutional capacity, management performance, organiser structure and communication channels, sources of pollution and sloop of the waste waters specific for users, hidromorphologic pressure, evolution of the water supply and request, normative for the prevention and full control of pollution, protected areas. In this step will be study, also: the facilities of treatment and purification, water price and the settlement regarding the quality, environment particularities (clime, geography, topography, water resources), field use, demographics data (actual state and tendency), ecological and hydro geological limited conditions. All these studies will be considered in the context of the national and international legislation.

5. **PN II-72-156/2009**, acronim- NANO-ZEOREZID: The use of some zeolitic materials functionalised with TiO_2 nano crystals for waste water treatment in the view of these reuse.

Value:9.200 LEIDirector:Lecturer Ph eng. Florica MANEAMembers:Prof. Ph. eng. Georgeta BURTICAPhd eng. Aniela POPPhd eng. Cristina PROCAPhd eng. Adriana BEBESELEA

FIELD DESCRIPTION

The use of some functionalized zeolitic materials with TiO_2 nano crystals for residual waters purification in the view of their reuse in the production process trough the combination of the advanced catalytic oxidation process with the electro oxidation process, or the involve of the TiO_2 in the process of photochemical and photo electrolytic purification.

ACTIVITIES AND RESULTS

Studies of scientifically reference material regarding the synthesis and applying of the zeolitic materials functionalised with TiO_2/TiO_2 nano crystals doped with metallic and non metallic ions, electrochemical degradation and integration of those two processes in the waste waters treatment with the purpose of their reuse.

6. PN II -71-026, Complex researches regarding the obtaining and the magnetically properties of the systems of ferromagnetic nanoparticles of surfactant/ un surfactant $CodFe_{3}-dO_4$ and biocompatibility with potential applying in cancer therapy.

 Value:
 0,000 RON

 Director:
 Prof. Ph. Mircea STEFANESCU

 Members:
 Assist. Ph. Eng. Marcela STOIA

 Assist. Ph. Eng. Monika SIMON
 Phd student eng. Thomas DIPPONG

FIELD DESCRIPTION

The project has like objectives the obtaining of the oxides systems $Co_xFe_{3-x}O_4$ under nano particles forms of various dimensions and their surfactation with biocompatible surfactants in the view of their use at the treatment of cancerous tumours. For the obtaining of the magnetic nano particles are used two unconventional methods of synthesis: the method of the thermal decay of the precursors of type carboxylic and the co precipitation method. Is followed the establishment of the synthesis

conditions needed for the obtaining of the magnetic nanoparticles of various dimensions, and also the study of their magnetical properties function of the medium diametere o0f the nano particles. The magnetic nano particles which will present adequate magmnetic properties will be surfatated and tested in the view of their use in the tumours treatment.

ACTIVITIES AND RESULTS

2 ISI paper accepted for publishing in JTAC two papers presented at the International conference of Thermal Analyse and Calorimetric, Brasilia 2008.

A PhD thesis sustained public in December 2008 on the project them. Synthesis of the nano materials type $CoxFe_{(3-x)}O_4$ with controlled magnetic properties.

PhD RESEARCH ACTIVITIES

1. Prof.dr.eng. Aurel IOVI, PhD Supervisor in *Chemical Engineering*

PhD students:

- Eugen Lungu: The use of activated oxidants in the waters treatment domain
- Dalila Marşavina: The studies of the equilibriums from the undergrounds waters in the view of the use of these as drinkable waters
- Dan Roşu: The behavior of the complex combinations with microelements in the obtaining process of the fertilizers
- Monica Ihoş: Unconventional technologies of elimination from water of some specific pollutants
- Cornel Bogatu: Specific technologies in the water technology
- Daniela Micu: The study of the toxic compounds elimination processes from rural waters sources
- Adrian Gheorghe Rus: The study of the obtaining processes of the active principles from medicinal plants and their characterizations
- Ioan Macarie: Contribution to the synthesis of some amino – organic – phosphoric with biological applied
- Valeria Rus: Studies regarding the sludge treatment from the local purification plant in the view of put in good use or elimination
- Mihaela Maria: Studies regarding the control and effect of the exposure to hard metals in the professional and unprofessional medium
- Florina Popa: Contributions to obtaining and using antiseptic agents based on synergetic mixture

2. Prof.dr.eng. Georgeta BURTICĂ, PhD Supervisor in *Chemical Engineering*

PhD students:

- Amalia Corina Macarie: Contributions at the ecotechnologies elaboration for the metallic ions recovery from the used electrolyte
- Petre Vili Furdui: Studies regarding the monitoring and characterization of the drinking water resources from the Romania's west region

- Nicoleta Luminița Jurj: Contributions regarding improvement of the municipal wastewater treatment technology for fall in with the European Normative
- Elena Gabriela Cical: Studies concerning the improvement of drinking water quality results from accumulation lake
- Mihaela Toader: Considerations regarding municipal wastewater treatment processes improvement
- Cristina Proca: Water decontamination technologies used new composite materials based on inorganic salts
- Ioana Maria Corb: Studies regarding the production and the characterization of new alumina silicate materials with utilization in ecotechnologies
- Daniela Ronamina Sonea: Drinking water treatment technology improvement
- Pisoi Ilie: Contributions regarding the improvements of the drinkable technologies of waters
- Puiulet Mihaela: Considerations regarding municipal wastewater treatment processes improvement
- Remes Adriana: Use of some zeolite materials functionalizated with TiO₂ nano crystals doped./undoped with metals/non-metals ions for wastewater treatment
- Damian Teodora: Studies regarding unconventional technologies elaboration for water treatment.
- Tudur Teodora: Studies regarding nitrites/ nitrates removal from underground water
- Baciu Ana Maria: Electromechical metods for quatitative evaluation for water polutants
- Motoc Sorina: Electro oxidation process application in water treatment technologies
- Masu Smaranda: Studies regarding appling of coagulation process for drinkable water obtaining.

3. Prof.dr.eng. Dumitru BECHERESCU, PhD supervisor in *Materials' Science and Engineering*

PhD students:

- Adriana Calapod: Concrete as an immobilization factor for some polluting materials
- 4. Prof.dr.eng. Ioan LAZĂU, PhD Supervisor in *Materials' Science and Engineering*

PhD students:

- Alexandru Orban: Technological parameters optimization for obtaining super-aluminous products
- Mariana Suba: The use of the unconventional methods in synthesys of some mineralogic compounds and solid solution for ciment chemistry

- Babuta Roxana: Synthesis of oxide compounds via Pechini method
- Ciobanu Cristina: The role and action mechanism of additives in dry mortars

5. Prof.dr.eng. Nicolae VASZILCSIN, PhD Supervisor in *Chemical Engineering*

PhD students:

- Mircea Dan: Metal removal from residual water in electrochemical reactor with vibrating electrodes
- Ana Maria Dabici: Nano particles type TiO₂ with photocatalitic activity
- Doru Buzatu: Electro catalise based on niobium
- Dan Rujan: Appling of the technologies of fracture theory in Galvan technique.
- Paula Sfirloagă: Materials for solar cells
- Ştefan Dănică Novaconi: Solar cells with TiO₂ and dyes
- Vaduva Constantin Claudiu: Corelation between the electronic structure of lever agents and double layer capacity
- Iorga Mirela Ioana: Metals removal from dilute solutions

6. Prof.dr.eng. Zeno GROPSIAN, PhD supervisor in *Chemical Engineering*

PhD students:

- Bors Nicu: "The investigation of some chemical products influence on the improvement of liquids flow"
- Ciobotaru Leopold: "Contributions to the filtering technology"
- Frigura (Panescu) Mihaela: "Contributions to the study of the solid-liquid separation processes"
- Pop Nadia: "Advanced methods for gases purification"

7. Prof.dr.eng. Delia Perju, PhD supervisor in *Chemical Engineering*

PhD students:

- Calisevici Mirela: Quality Performances Improvement of a Food Process Line Using Advanced Optimal Process Control
- David Ioana Elena: Study Regarding the Process Control and Optimization Possibilities of Technological Processes Applied in Fibre Glass Technology
- Manea Adela: Contributions to the Quality Improvement of Cosmetics Products
- Osiceanu Antoaneta: Contributions to Optimisation of Asphaltic Cationic Emulsion Technology.
- Lal Astrid: Contributions to the Elimination Process Improvement of Pollutants Resulted from Railway Units Activity
- Pamfiloiu Mirabela: Contributions to the Improvement of an Electro thermal Gas Flow meter Performances Using Analogue-Numerical Systems
- Cicoare Eugeniu: Contributions to the Implementation Possibilities of Low Pressure Equipments in Physical-Mechanical Test-

Installations Used in the Chemical Technology of Leather

- Firczak Monica: Contributions to the Study of Neural Networks Applied in Chemical Engineering
- Ordodi Valentin: Designing of a micro reactor for the obtaining of the STEM cells
- Draghici Loredana: Contributions regarding the environment protection for the nocive effects of the hazardous substances resulted after the accidental technologies using the mathematical modelation and numeric simulation.
- Clavac Bogdan: Impact evaluation study on the environment induced by the refuse dumps derived from coke-chemical plants by means of mathematical modelling techniques
- Crivineanu Marilena: Study of heavy metal emission processes in running waters by mean of mathematical modelling methods

8. Prof. PhD Mircea ŞTEFĂNESCU, PhD Supervisor in *Chemistry*

PhD students:

- Vlăzan Paulina: Oxides nano materials used as environment sensors
- Barbu Mirela: The preparation and characterisation of some nanocomposites based on transitional metal chromites
- Tita Bogdan: Contributions on the study of the compatibility and thermal stability of some drugs from NSAID class. Synthesis of their coordination compounds

9. Prof. PhD Rodica PODE, PhD supervisor in *Chemical Engineering*

PhD students:

- Ilinoiu Elida-Cristina: Contributions to the development of hybrid advanced oxidation processes for the degradation of persistent organic pollutants
- Colar Liliana Andreea: Improvement of specific industrial effluents treatment technology by applying photocatalytic heterogenous processes

10. Prof. PhD Corneliu DAVIDESCU, PhD supervisor in *Chemical Engineering*

PhD students:

- Stefanescu Oana: Metode noi de obtinere a nanomaterialelor pe baza de g-Fe₂O₃
- Kakasi Zsurka Sandor; Noi bioproduse prin valorificarea acizilor hidroxialcanoici
- Croitoru Alina Ramona: Utilizarea lipazelor impobilizate pentru sinteza esterilor de oligo-si polizaharide
- Corici Livia Nicoleta: Utilizarea alcalazei imobilizate in sinteza peptidelor
- Rafaila Madian: Studiul relatie structurareactivitate chimica in chimia organica
- Ardelean Radu: Specii chimice heterogenizate prin grefare pe matrici polimere

Peli Beata Monika: Protectia si depoluarea apelor utilizand specii chimice grefate pe suporturii macromoleculare

PhD THESIS SUSTAINED

- 1. Eleonora Marian: *Complexes of transition elements with medicinal substances,* PhD supervisor: prof. dr. Ilie Julean
- 2. Claudia Morgovan: *The reuse of the metals ions* from galvanic industry wastes under fertilizers with microelements, PhD supervisor: prof. dr. eng. Aurel Iovi
- 3. Angela Magda: Studies about some oxygenate compounds of boron with applied in fertilizers technologies with microelements, PhD supervisor: prof. dr. eng. Aurel Iovi
- 4. Laura Cocheci: Oxidative chemical processes for soil decontamination, PhD supervisor: prof. dr. eng. Aurel Iovi
- 5. Carmen Lazau: Studies regarding the characterizations and the use of some nano materials of type TiO_2 in the ambient environmental decontamination, PhD supervisor: prof. dr. eng. Aurel Iovi
- 6. Cornelia Elena Ratiu: *New materials in drinking water treatment technology*, PhD supervisor: prof. dr. eng. Georgeta Burtică
- 7. Ianosev Silvana: Using unconventional synthesis methods in the preparation of some oxide compounds in SiO2-Al2O3-MxOy systems, PhD supervisor: prof. dr. eng. Ioan Lazău
- Radu Nicolae Bănică: Solar cells based on CuInS₂, PhD supervisor: prof. dr. eng. Nicolae Vaszilcsin
- Harieta Pîrlea: Contibution to the simulation and modeling of chemical processis for reduction of nitrogen dioxide emissions, PhD supervisor: prof. dr. eng. Delia Perju
- 10. Marinescu Sorin: *Contributions to the Optimization Possibilities of a Waste Incineration Plant*, PhD supervisor: prof. dr. eng. Delia Perju.

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RESEARCH CENTRE SYNTHESIS AND APPLICATIONS OF ORGANIC AND MACROMOLECULAR COMPOUNDS - S.A.O.M.C.

GENERAL PRESENTATION

Synthesis and Applications of Organic and Macromolecular Compounds (S.A.O.M.C.) is a research centre, type C, which has been evaluated and approved by CNCSIS. The Centre was created in 2002, in accordance with the CNCSIS certificate, nr. 47/4.12.2003. The director of the Centre is Assoc.prof.dr.eng. Mihai Medeleanu.

MAIN ACTIVITIES

The Center performs research activities in domains such as:

- BioNanoMaterials obtaining, characterization and applications of the biocompounds and biosystems/cyclodextrins or liposomes nanoparticles
- Drug Design and Synthesis molecular modeling, SAR, QSAR, virtual high throughput screening, docking, synthesis, analysis and applications of drugs
- Natural Food Flavours and Spices isolation, purification, stabilization, conditioning, and characterization of natural extracts or compunds used as flavours and sipces
- Perfumes and Cosmetics obtaining, stabilization, characterization of natural biosystems with applications in perfumery and cosmetic industry
- New methods in organic synthesis
- Studies on structure-properties relationship using the topological model of organic molecules
- Structured packings and their applications in systems with chemical reaction

- Synthesis and characterization of PVC plasticizers
- Oligomers with functional groups
- Chemistry and technology of drugs and pesticides
- Chemistry and technology of dyestuffs, and textile auxiliaries
- Process control equipments for research plants in chemical industry
- Control systems using computers for researching plants and low tonnage plants in chemical industry
- Intensive methods for the exoneration of soil from radioactive minerals exploitation and processing areas in the condition of natural disasters or entropic accidents
- Mathematical modeling and numerical simulation of environmental pollution and depollution processes
- Modeling, simulation and process control
- Magnetic Fluids: Preparation, Characterization and Applications
- Heat transfer organic agents
- Unit processes
- The Intensification of Transfer Processes
- Rheological characterization of the substances

CONTACT

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RESEARCH FIELDS

BioNanoMaterials

Keywords: bioactive compounds, drugs, natural compounds, nanoparticles, nanocapsules, cyclodextrins, liposomes, scanning electron microscopy, transmission electron microscopy, thermogravimetry, differential scanning calorimetry, preparative liquid chromatography

Drug Design and Synthesis

Keywords: drugs, drug design, total synthesis, semisynthesis, biosynthesis, quantitative structureactivity relationships, virtual high throughput screening, docking, gas chromatography, preparative liquid chromatography, high pressure liquid chromatography

Natural Food Flavours and Spices

Keywords: flavor, flavour, aroma, food, odorant, spice, biosynthesis, biotechnology, extraction, natural food additives, gas chromatography, GC, analytical high pressure liquid chromatography, HPLC, spectrometry, spectrofotometry, sensory analysis, statistical multivariate analysis, PCA, HCA

Perfumes and Cosmetics

Keywords: perfumes, cosmetics, odorants, terpenoids, biosynthesis, biotechnology, extraction, toiletries, essential oils, volatile compounds, design of perfumes, gas chromatography, GC, analytical high pressure liquid chromatography, HPLC, spectrometry, spectrofotometry, olfactometry, statistical multivariate analysis, PCA

> New methods in organic synthesis

Keywords: synthesis of organic compounds, carbonic acid derivatives, sterically hindered phenols with antioxidant activity, structure determination by NMR, biocatalysis of organic reactions

Studies on structure-properties relationship using the topological model of organic molecules

Keywords: topology, graphs, structure-properties relationship (SAR), size and shape of molecules, van der Waals volume and surface

Structured packings and their applications in systems with chemical reaction

Keywords: static mixers, motionless mixers

Plasticizers for polymers

Keywords: plasticizer, plasticizing

Synthesis and characterization of PVC plasticizers

Keywords: PVC-plasticizer

Oligomers with functional groups

Keywords: oligomer, functional group, reactive oligomers

Chemistry and technology of drugs and pesticides

Keywords: drug, pesticides, chemistry, technology, semi synthesis, agriculture

Chemistry and technology of dyestuffs, and textile auxiliaries

Keywords: dyes, dye accelerators, dispersants, textile auxiliaires

Process control equipments for research plants in chemical industry

Keywords: measuring, control devices

Control systems using computers for researching plants and low tonnage plants in chemical industry

Keywords: process control, research and low tonnage plants

Intensive methods for the exoneration of soil from radioactive minerals exploitation and processing areas in the condition of natural disasters or entropic accidents

Keywords: Climate changes, pollution, risk, sustainable chemistry, modeling

Mathematical modeling and numerical simulation of environmental pollution and depollution processes

Keywords: modeling, simulation, environmental protection

Oily compounds extraction from waste waters using magnetic fluids

Keywords: extraction, magnetic fluid

The Performance of Columns with Structured Packings

Keywords: wet ability, specific surface

Researches in BIONANOMATERIALS

Obtaining and analyses methods on the bioactive systems/cyclodextrins compounds and and liposomes micro/nanoparticles. The bioactive compounds used for nanoencapsulation are: drugs, natural compounds with biological activity (i.e. alkaloids and flavonoids, volatile oils), perfumes and cosmetics, natural food additives (i.e. natural flavors, natural colorants). These products have excellent properties in comparation with the starting materials: oxidative, thermal stability, protective properties against radiations, controlled release of the bioactive compounds, hydrosolubilization of hydrophobic biocompounds, masking of the unpleasant taste and odors, easily handling of the powdery bionanomaterials.

The methods used for obtaining of the bionanomaterials are: crystalize from solution, spray-drying, spray-chilling, fluidized bed, by mixing or melting, by ultrasonication. The main methods of separation-[urification and analyses are: preparative liquid chromatography (preparative HPLC), scanning electron microscopy (SEM), transmission electron microscopy (TEM),

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thermogravimetry (TG), differential scanning calorimetry (DSC).

RESEARCH TEAM

Daniel Hădărugă, Geza Bandur, Gerlinde Rusu, Iulia Pînzaru, Volica Damșa

Researches in DRUG DESIGN and SYNTHESIS

Design of new compounds with potential drug properties and synthesis of hits. The methods used for drug design are: molecular modeling of the known compounds, qualitative and quantitative structure-activity relationship studies (SAR and QSAR), virtual high throughput screening (VHTS), molecular docking of the predicted drugs.

The hits selected by drug design are obtained by known methods (total synthesis, semi-synthesis, biosynthesis), separed and analyzed by modern methods (preparative liquid chromatography – preparative HPLC, liquid and gas chromatography – HPLC and GC, ¹H- and ¹³C-NMR, X ray diffraction, UV-VIS, IR, MS spectroscopy) and further evaluated as drugs.

RESEARCH TEAM

Daniel Hădărugă, Mihai Medeleanu, Geza Bandur, Gerlinde Rusu, Iulia Pînzaru, Volica Damşa

Researches in NATURAL FOOD FLAVOURS AND SPICES

Developing new natural food flavours and spices with enhanced stability and bioactivity, more healty and with functional properties. The obtaining of food flavours and spices (especially those from the Romanian tradition) are realized by classical methods (non-aggressive, like hydrodistillation, hydroalcoholic or supercritical fluid extraction etc.). The analysis of these biosystems are realized by chromatographic (GC, HPLC, GC-O, TLC), spectroscopic (FT-IR, UV-Vis, NMR), and sensorial methods. The protection and controlled release of the natural bioactive compunds are realized by micro/nanoencapsulation in natural bioavailable matrices (like cyclodextrins and liposomes), and the analysis of these nanoparticles are realized by microscopic and thermal analyses (like, SEM, TEM, TG, DSC).

RESEARCH TEAM

Francisc Peter, Daniel Hădărugă, Geza Bandur, Gerlinde Rusu, Iulia Pînzaru, Volica Damșa

Researches in PERFUMES AND COSMETICS

Design and evaluation of new perfume and cosmetic formulations. The main ingredients from perfume or cosmetic formulations are obtained from natural resources (especially from the traditional herbs) by classical methods (hydrodistillation, hydroalcoholic or supercritical fluid extraction etc.). The analysis of these biosystems are realized by gas chromatography (GC-FID, GC-MS, GC-Sniffing etc.), liquid chromatography (RP – HPLC – UV – Vis / MS) spectroscopic methods for bioactive compounds (FT-IR, UV-Vis, NMR), and sensory analysis. The protection and controlled release of the natural odorant compounds from natural bioactive systems are realized by micro/nanoencapsulation in natural bioavailable matrices (like cyclodextrins and liposomes), and the analysis of these nanoparticles are realized by microscopic and thermal analyses (like, SEM, TEM, TG, DSC).

RESEARCH TEAM

Daniel Hădărugă, Mirabela Pădure, Gerlinde Rusu, Iulia Pînzaru, Volica Damșa

Researches in NEW METHODS IN ORGANIC SYNTHESIS

Synthesis of organic compounds (carbonic acid derivatives, phenolic antioxidants, amino acids and peptides) using new methods or reagents: single electron transfer reactions, triphosgene as a low toxic and easy to handle substitute of phosgene, isatoic anhydrides, enzymes obtained by biosynthesis or extraction (aminoacylase, protease, lipase).

The chemistry of organic derivatives of carbonic acid is the traditional field of our Department, pioneered by Professor Giorgio Ostrogovich. Studies in the field of synthesis of chlorocarbonates, carbonyl chlorides, carbamates, carbonates, ureas, aryl cyanates, isocyanides and heterocyclic as well as kinetics and mechanisms of reactions of carbonic acid derivatives were performed. Since 1980 synthesis of phenolic antioxidants, studies of biocatalytic processes in organic synthesis and structure determination of organic compounds by NMR spectroscopy were also investigated.

RESEARCH TEAM

Carol Csunderlik, Mihai Medeleanu, Marius Milea, Francisc Peter

Researches in STUDIES ON STRUCTURE-PROPERTIES RELATIONSHIP USING THE TOPOLOGICAL MODEL OF ORGANIC MOLECULES

The topological model, as an application of graph theory in chemistry is a useful tool for quantification of molecular structure and has been largely used in the last years, due to its simplicity and good correlation results in studies concerning the shape and size of molecules and structure-properties relationship for many classes of compounds.

By applying the topological model to organic molecules, information's like the number of atoms and the connectivity's are compressed in numbers named topological indices. These can be correlated with physical and chemical properties and biological activities and are also used to describe the shape and size of molecules. Better correlation coefficients were obtained when certain heteroatom were included into topological model (halo derivatives, oxygen and sulphur derivatives and local anesthetics). Van der Waals surface and volume of organic molecules were also performed using the Monte Carlo algorithm.

RESEARCH TEAM Mihai Medeleanu, Daniel Hădărugă

Researches in STRUCTURED PACKINGS AND THEIR APPLICATIONS IN SYSTEMS WITH CHEMICAL REACTION

The structured packings (former name: static mixers or motionless mixers) increase the mixing efficiency in all flow regime, but any other device does not equalize their performances in the laminar flow regime. Their application in all types of reactive systems (homogeneous or heterogeneous) has started several years ago and is in a continuous expansion. Recently, catalysts supported on static mixers are commercially available.

Since 1986, different applications were developed (e.g. reactor for hydrogenation of fatty oils, CO_2 absorption in monoethanolamine solutions). Theoretical studies include: investigations concerning the mixing mechanism in columns equipped with Sulzer SMV type static mixers; influences of main parameters on the size and distribution of the droplets formed in column fitted with structured packings; analysis of gas holdup and solid distribution in three phase gas-liquid-solid reactors equipped with different motionless mixers in order to grow the liquid phase conversion in slurry bubble columns.

RESEARCH TEAM

Lucian Rusnac, Sabina Niţu, Carmen Rusnac

Researches in PLASTICIZERS FOR POLYMERS

The undertaken research aims to correlate the structure and the plasticizing properties, both permanent and temporary of certain polymers, belonging to new series of chemical compounds.

More than 100 new substances have been synthesized, described and assessed. Within the same framework of activity, there has been a practical and theoretical concern for the problems of both permanent and temporary plasticizing of polar polymers, thus enabling the drawing of conclusions with a view to industrial applications and to new correlation of the structure and the plasticizing properties. The research is represented by more than 60 scientific papers and research agreements.

RESEARCH TEAM

Ionel Manoviciu, Geza Bandur, Gerlinde Rusu

Researches in SYNTHESIS AND CHARACTERIZATION OF PVC PLASTICIZERS

Many high molecular weight materials, organic and inorganic, are benefited by plasticizers, yet our major emphasis is on organic plasticizers for synthetic organic polymers and particularly for PVC.

Since 1970 we are concerned with the synthesis and characterization of some new ester type PVC plasticizers, namely "direct" plasticizers derived from a diacid and "reversed" plasticizers derived from a diol esterifies with monoacid. Taking into account the fundamental technological and theoretical parameters (as the Flory-Huggins interaction parameter χ and the Hildebrand solubility parameter δ) it becomes possible to correlate the structure of the models involved with their real effectiveness in PVC compounds.

RESEARCH TEAM Liviu Mirci, Sorina Boran, Sergiu Curelea

Researches in OLIGOMERS WITH FUNCTIONAL GROUPS

Synthesis and characterization of some lowmolecular polymers of different structure, containing two or several functional groups capable of undergoing some subsequent chemical transformations

Synthesis, characterization and application of dimethacrylates as reactive plasticizers for poly (vinyl-chloride). Synthesis and characterization of functional oligomers under non-stoichiometric conditions with a total conversion (α, ω -dihydroxy-polyesters). Chemical modification of polyethylene oligomers.

RESEARCH TEAM

Ionel Manoviciu, Geza Bandur, Gerlinde Rusu

Researches in CHEMISTRY AND TECHNOLOGY OF DRUGS AND PESTICIDES

Synthesis, analysis and testing of total and semi synthetic drugs, odorants and pesticides for human use and agricultural applications

Studies in this field have been started since 1950 at the Faculty of Industrial Chemistry of Technical University Timisoara (former Polytechnic Institute of Timisoara). This activity was finalized in books, manuals, journal papers, patents and research programs for micro production and industry.

RESEARCH TEAM

Constantin Daescu, Alfa-Xenia Lupea, Daniel Hădărugă, Mirabela Padure, Zlatimir Stanoiev.

Researches in CHEMISTRY AND TECHNOLOGY OF DYESTUFFS, AND TEXTILE AUXILIARIES

Synthesis of organic dyestuffs, dyeing accelerators and dispersants.

The researches undertaken have been concerned with the study of separating components in organic dyes synthesis. Synthesis of some new substantive cationic dyes used in finishing natural and synthetic yarns and fibers has been studied. Syntheses of some key intermediates for organic dye technologies have also been performed.

RESEARCH TEAM

Simona Popa, Ioan Macarie

Researches in PHYSICAL CHEMISTRY. CHEMICALLY ACTIVE SPECIES GRAFTED ON POLYMER-SUPPORTS

Preparation and investigation of chemically active species (catalysts, reagents, substrates, enzymes, polycationic biocides) grafted on polymer-supports (styrene-divinylbenzene copolymers, polyethylene glycol) acting as "hybrid-phase" systems. Studies on the structure-activity relationship. Synthesis and testing of multifunctional or multistep recyclable and reusable catalysts.

Since 1982 the research program in the field was focused on the synthesis of the new types of polymer ligand homologous of Schiff bases, hydrazones, oximes and azines by polymeranalogous reactions, synthesis of polymer-grafted tertiary heterocyclic amines acting as "hybridphase" biomimetic catalysts similar to chemotripsine and studies of the kinetics, mechanism and structure-activity relationship in a test reaction of activated esters hydrolysis. A new kinetic model of the nucleophile bimolecular substitution using phosphonium and/or ammonium salts grafted on polymer-supports as phase-transfer catalysts was proposed.

RESEARCH TEAM

Corneliu Davidescu, Erika Reisz, Radu Ardelean

RESEARCH PROJECTS

1. CEEX CHIROMAR 2CEX06-11-30/25.07.2006: Molecular Chirality: Determination of Enantiomeric Excess and Absolute Configuration by Nuclear Magnetic Resonance Spectroscopy (NMR) and Application to Bioactive Compounds and Intermediates in Fine Synthesis.

Value:	92.000 RON
Director:	Prof. dr. Carol CSUNDERLIK
Members:	Lect. dr. Vasile BERCEAN
	Assoc. prof. dr. Francisc PETER
	Assist.dr. Valentin BADEA
	Assist. dr. Monika SIMON
	Ph.D student Ana Cristina ZARCULA

FIELD DESCRIPTION

Preparation and Characterisation of Moleculat Chirality of Some Intermediates and Bioactive Compounds by Magnetic Resonance Spectroscopy (NMR).

ACTIVITIES

Stereoselective Synthesis of Some Chirals Betaaminoacids. Chiral separations.

- enantioselective acylation of secondary alcohols by sol-gel etrapped lipases
- determination of enantiomeric ratio of chiral esters obtained by gas chromatograpy using a chiral column
- obtaining of chiral oxazolidinone as precursors for beta-aminoacids synthesis.

2. CEEX RMNSTAR 2CEX06-11-41/25.07.2006: Adaptation of Sequences of NMR Pulses, Elaboration of Multicentre-type Ttests and On-line Interconnecting of the Superconductive NMR Spectrometers in Romania.

Value:	60.000 RON
Director:	Prof. dr. Carol CSUNDERLIK
Members:	Prof. dr. Corneliu-Mircea
	DAVIDESCU
	Assoc. prof. dr. Mihai MEDELEANU
	Assoc. prof. dr. Petru NEGREA
	Assist.dr. Valentin BADEA
	Assist. dr. Monika SIMON
	Assist. Radu ARDELEAN
	Assist. Narcis DUTEAN

ACTIVITIES

Elaboration of multicentre-type tests and on-line interconnecting of the superconductive NMR spectrometers in Romania.

3. PN-II IDEI Grant 268/01.10.2007: New bioproducts by valorization of microbial hydroxyalkanoic acids

Value: 208.820 RON

Director: Prof.dr.eng. Francisc PETER Members: Prof.dr.eng. Corneliu DAVIDESCU Prof.dr.eng. Carmen BOERIU PhD student eng. Cristina ZARCULA PhD student eng. Sandor Balazs KAKASI-ZSURKA

FIELD DESCRIPTION

Industrial biobased products have an increasing potential in the chemical and material industries. The diversity of biomass feedstocks like sugars, oils, proteins, or lignocellulosics, combined with the numerous biochemical and thermochemical conversion technologies, can provide a diversity of polymers, lubricants, products as solvents. adhesives. herbicides, and pharmaceuticals. Polyhydroxyalkanoates (PHAs) are polyesters of various hydroxyalkanoates that are synthesized by These polymers are accumulated bacteria.

intracellularly to levels as high as 90% of the cell dry weight and are stored as granules, to act as carbon and energy reserve.

The objectives pursued by the fulfilling of this project are based on the current stage of knowledge on PHA and their transformations. Considering the large interest for this field, it is presumable that a series of such products, obtained from either microorganisms or plants, will be available at reasonable prices and in large quantities. In these conditions, the development of knowledge on this field and the broadening of the area of applications by the manufacture of new bioproducts shlould have a strong impact on the development of new technologies based on renewable materials. This project has an interdisciplinary character, as it aims the investigation of biocatalytical processes, optimization of the functionality of enzymes, synthesis and physico-chemical characterization of organic bioproducts and biopolymers.

ACTIVITIES

In the year 2008 the activities were focused on the following reasearch topics:

- Survey of the recent scientific literature concerning polyhydroxyalkanoate hydrolysis and synthesis of β-butyrolactone copolymers.
- Chemical and enzymatic hydrolysis of PHA's
- Biocatalytic synthesis of 3-hydroxybutyric acid esters using lipases, determination of optimal reaction conditions, identification and characterization of reaction products
- Immobilization study of microbial lipases
- Experimental protocol for β-butyrolactone copolymers synthesis and characterization of reaction intermediates and products.

4. PN2 21077/14.09.2007: *Biofuels obtained by* valorization of cellulosic residues in an integrated chemo-enzymatic system.

Value:167.731 RONDirector:Prof.dr.eng. Francisc PETERMembers:Prof.dr.eng. Dumitru TUCUProf.dr.eng. Dumitru MNERIELect.dr.eng. Marius GHEJUAssist.drd.eng. Cristina ZARCULALect.dr.eng. Titus SLAVICILect.dr.eng. Dinu GUBENCU

FIELD DESCRIPTION

Bioethanol manufacture is a very complex issue, resulting from the diversity of the raw material and difficulties of set up the optimal parameters for every process step.

This project is targeted on valorization of residual lignocellolosic biomass resources by conversion to bioethanol, using an optimal combination of chemical and biocatalytic steps.

The main objectives pursued by this project are: manufacture of laboratory equipments for

pretreatment of lignocellulosic materials, to ensure maximum efficiency of the following hydrolysis step; optimization of the pretratment method based on the composition of cellulosic biomass; investigation of enzymatic hydrolysis of cellulose and cellolose-containing substrates, using the new generation of highly efficient cellulolytic enzymes comercially available (Genencor, Novozyme); evaluation of immobilization possibilies of cellulases, for possible multiple reuse; study of cellulosic sugars fermentation and optimization of bioreactor parameters for simultaneous fermentation of hexoses and pentoses, avoiding inhibitions: investigation of simultaneous saccharification and fermentation; isolation and characterization of the obtained bioethanol, and evaluation of biofuel properties.

ACTIVITIES

The main activities issued for 2008 have been:

- Physico-chemical characterization of the raw materials from cellulosic biomass
- Manufacture of a laboratory eqipment for mechanical pretreatment by grinding of solid cellulosic residues
- Study of pretreatment methods of cellulosic biomass (acid, microwave) and analysis of the resulted products
- Enzymatic hydrolysis of cellulose and cellulose containing biomass hydrolyzates.

5. CEEX MANANTECH 82/2006, Organophosphoric-like hybrids with special properties

Value: 20.000 RON

Director: Assoc.prof.dr.eng. Geza BANDUR Members: Lect.dr.eng. Simona POPA Assist.dr.eng. Gerlinde RUSU

6. PN2 PC 72152/1.10.2008: Synthesis and investigation of biodegradable polymers based on polylactic acid, with applications in medicine (BIOPLAST)

Value: 0 RON *Director:* Assoc.prof.dr

Director: Assoc.prof.dr.eng. Geza BANDUR Members: Prof.dr.eng. Francisc PETER Assist.dr.eng. Gerlinde RUSU PhD Stud. eng. Sandor KAKASI-ZSURKA

FIELD DESCRIPTION

One of the main contemporary scientific challenges is discovery and manufacturing of new ecologically friendly, biodegradable and biocompatible polymers which could replace the existing polymeric materials.

Polylactic acid is such a material, extensively studied for industrial and biomedical applications. Its biocompatibility is owed to lactic acid, the degradation products which can be metabolized. The main objectives of this project are the synthesis and characterization of polymeric structures with new properties, based on racemic and/or enatiomerically pure (L-form) lactic acid. Policondensation reactions of lactic acid monomers will be investigated by non-catalyzed reactions at 100-300°C, or in microwave conditions. Inclusion of other monomers like as diphenyl-methyl isocyanate and/or ethyleneglycols in the polymer chain will be also studied to obtain new copolymers with improved properties and extended applications.

Oligomer mixtures and multibloc copolymers will be characterized by specific methods as sizeexclusion chromatography, magnetic resonance spectrometry, spectrometry, mass infrared spectroscopy, thermal analysis. The mechanistic and elastic properties of the new biopolymers will be also evaluated, compared to well-known materials (polivinvl polymeric chloride. polyethylene, polyurethanes), as well as the degradation and biodegradation properties.

ACTIVITIES

Survey of the recent scientific literature concerning biodgradable polymers holding ester likages.

7. CEEX 2-CEEX06-11.57 (2006-2008), Modern Technology for Pyrazin-2,3-dicarbixylic acid synthesis – an intermediate for drug synthesis

Value: 205.000 RON Director: Assoc. prof. dr. eng. Mihai MEDELEANU

Members: Prof. dr. eng. Nicolae VASZILCZIN Prof. dr. eng. Francisc PETER Assoc. prof. dr. eng. Andreea KELLENBERGER Asist. eng. Zlatimir STANOIEV Asist. Mircea DAN PhD Stud. eng. Oana Raluca POP

FIELD DESCRIPTION

Studies concerning new electrochemical methods for synthesis of pyrazine dicarboxylic acid.

ACTIVITIES

- Building a data base for electrochemical oxydative methods applied in organic chemistry.
- \blacktriangleright Mn⁷⁺ based intermediate synthesis.
- Optimal reaction path analysis and kinetic studies.
- Stability of MnO_4^2/MnO_4^2 redox couple.
- Quinoxaline oxydation by the above intermediate.
- Methods for analysis. Technology setup.

8. P4 – Priority Domains Partnership, Reasearch grant 52-145 (2008-2010), *Antioxidant and*

Hypoglycemia Food Supplements with Anthocyanidin Structure (SAHASA)

Value:	200.000 RON
Director:	Assoc. prof. dr. eng.
	Mihai MEDELEANU
Members:	Assist. dr. eng. Valentin BADEA
	Assist. dr. eng. Monika SIMON
	Asist. eng. Zlatimir STANOIEV
	Asist. eng. Mircea DAN
	PhD Stud. eng. Oana Raluca POP
	PhD Stud. eng. Beniamin PINTEA
	PhD Stud. eng. Ioana POPA

FIELD DESCRIPTION

This project is focused on the evaluation of potential antioxidant activity as well as hypoglicemia effects of compounds with anthocyanidin structure obtained from natural extracts.

ACTIVITIES

- Identification and dosage of possible antioxydant activity and hypoglicemia effects components from inland plant species.
- Technology setup for biological active components extraction
- Physico-chemical methods for exactly identification of structures and compositions of biological active mixtures.
- In vitro testing of biological activity.

9. PN2 PC-41070 / 18.09.2007, Action and stressprotecting / immunostimulating effects of some new bioactive materials (IMUNO-NANOMAT)

Value: 100.000 RON

Director: Lect.dr.eng. Daniel-Ioan HĂDĂRUGĂ Members: Assoc.prof.dr.eng. Geza N. BANDUR Lect.dr.eng. Nicoleta G. HĂDĂRUGĂ Teach.assist.eng. Iulia A. PÎNZARU Tehn. Volica DAMSA

FIELD DESCRIPTION

In this project, the obtaining, analysis and application of the titanium dioxide (undopped and dopped with Au, Ag, Pt ions)/biocompatible /nanoparticles micro/ matrices micro and nanocapsules will be studied. Cyclodextrins, liposomes and other similar natural compounds (systems) will be used as encapsulation matrices. The biocompatible nanoparticles will be obtained by spray-drying, spray-chilling, fluidized bed, or ultrasonic methods. The analysis of the micro/nanoparticles will be realized by microscopical methods (SEM, TEM), termoanalytical (thermogravimetry, methods differential scanning calorimetry), X ray diffraction etc. The bionanomaterials will be evaluated from the stress-protecting and/or immuno-stimulating effects point of view.

ACTIVITIES

- Literature survey on the obtaining and characterization of micro/nanoparticles, especially containing metal oxides and metal ions;
- Experimental design of the micro/nanoencapsulation processes;
- Obtaining and characterization of the undopped TiO2/biocompatible matrices micro/nanoparticles;
- Obtaining and characterization of the Au, Ag, Pt dopped TiO2/biocompatible matrices micro/nanoparticles;
- Optimization of the micro/nanoencapsulation processes.
- 10. PN2 PC-62072/ 1.10.2008, Hepatoprotecting nanoparticles with enhanced bioavailability (Nano-HEPAT)
- Value: 326.750 RON
- *Director:* Lect.dr.eng. Daniel-Ioan HĂDĂRUGĂ *Members:* Assoc.prof.dr.eng. Geza N. BANDUR
- Prof.dr.eng. Francisc PETER Assoc.prof.dr.eng.M. MEDELEANU Lect.dr.eng. Andra TAMAS Teach.assist.eng. Gerlinde RUSU Teach.assist.eng. Iulia A. PÎNZARU PhD Stud. eng. Cristina ZARCULA Tehn. Volica DAMŞA MS Stud.eng. Radu PREJBAN MS Stud.eng. Ionut TANASE MS Stud.eng. Gabriel TOTH

FIELD DESCRIPTION

In this project, the obtaining (separation, purification), semi-synthesis, nanoencapsulation, analysis, and hepatoprotective evaluation of natural or modified biosystems or biocompounds from *Chelidonium, Berberis, Matricaria* species will be studied.

The obtaining of the hepatoprotective biosystems from Chelidonium, Berberis, Matricaria species will be realized by classical ethanol-water extraction, the extracts will be fractionated by preparative liquid chromatography, and evaluated from the hepatoprotective point of view. The extracts/fractions/natural compounds with the best activity will be used for the obtaining of cyclodextrin-like nanoparticles (or other encapsulation matrices). Furthermore, some active compounds will be chemically modified in order to increase the hepatoprotective activity and these compounds will be used for the obtaining of nanoparticles with enhanced bioavailability.

The analysis of the extracts/fractions/natural or modified compounds will be realized by GC (after derivatizing), HPLC, MS, NMR, FT-IR etc. The analysis of nanoparticles will be realized by microscopical methods (SEM, TEM, AFM), termoanalytical methods (thermogravimetry, differential scanning calorimetry), X ray diffraction, EDAX etc.

ACTIVITIES

- Literature survey on the obtaining and characterization of *Chelidonium*, *Berberis*, *Matricaria* extracts/main compounds, and on the obtaining and analysis of such bioactive compounds/cyclodextrin nanoparticles;
- Experimental design of the nanoencapsulation processes between bioactive compounds/ cyclodextrins;
- Obtaining and characterization of the Chelidonium, Berberis, Matricaria extracts/ fractions/bioactive compounds (with hepatoprotective activity);
- Obtaining and characterization of the bioactive compounds or extracts/cyclodextrin nanoparticles (with enhanced bioavailability on the hepatoprotection);
- Optimization of the nanoencapsulation processes.

PhD RESEARCH ACTIVITIES

1. Prof.dr. Carol CSUNDERLIK, PhD supervisor

PhD students:

- Nitu Sabina Violeta: Synthesis and Characterization of Some Pyrazole Derivatives
- Szöcz-Biro Emese: Synthesis of Functional Derivatives of Polyhydroxilic Compounds Using Biotransformation Reactions with Free or Immobilized Enzymes
- Pop Oana Raluca: Synthesis and Reactivity of Some Carbonylic Derivatives of Aromatic Heterocycles
- Şişu Ioana: Studies of the Synthetic Methods for Obtaining of Functional Derivatives of Aldoses
- Palani Adil: Thermal Decomposition of N-Carbamoil Derivatives of Cyclic Imides
- Ledeți Ionuț: Synthesis of functionalized mercapto-triazoles and use as ligands or compounds with potential biological activity
- Creangă Andreea Anda: Synthesis of heterocyclic mercaptans from azol class
- 2. Prof.dr.eng. Ionel MANOVICIU, PhD supervisor

PhD students:

- Homone Claudia-Gabriela: Contributions to study of rubber compound's composition for rolling bands and hard tire's flank
- Roşca Cristina: Interaction characterization of rubber-filling
- Mişcă Ruxanda Manuela: Researches about improvement of physico -mechanic characteristics of synthetics elastomers's compounds

- Uscătescu Maria Ramona: Contribution at study of rubber mixture's adherence at transport band's base
- 3. Prof. dr. eng. Alfa-Xenia LUPEA, PhD supervisor

PhD students:

- Lascu Anca: Study on the reaction of anomeric center of monosaccharides
- Condrat Dumitru: Obtaining of some plant extracts with antioxidant activity
- Grăvilă Corina: Synthesis of substituted Namides of aromates hydroxy-acids
- Crăşmăreanu Eleonora Cornelia: Synthesis and characterization of intermediates and colorants with amidic groups
- Vancea Valentina: Synthesis of some pyridine derivatives with potential biological activity
- Taloş Ioan: Synthesis and properties of some phosphonic acids and derivatives
- Costescu Corina Iuliana: Stabilizing of some bioactive principles from Compositae family plants by cyclodextrin nanoencapsulation
- Pleşa Carmen Manuela: Juniperus extracts: obtaining and uses in pharmaceutics, cosmetics, and food fields

4. Prof. dr. eng. Corneliu-Mircea DAVIDESCU, PhD supervisor

PhD students:

- Kakasi-Zsurka Sandor: Obtaining of some new bioactive compounds by modification of polyhydroxyalkanoates
- Corici Livia: Biocatalytic processes with immobilized enzymes by sol-gel method
- Croitoru Ramona: Synthesis of carbon hydrates oligomers and polymers by enzymatic catalysis
- Stefanescu Oana: FexOy type oxidic nanomaterials undispersed and dispersed in anorganic-organic matrices: synthesis, characterization, application
- Răfăilă Madian: Doctoral School
- Ardelean Radu Ovidiu: Doctoral School
- Peli Beata Monika (căs. Cioplea): Doctoral School
- 5. Prof.dr.eng. Lucian RUSNAC, PhD supervisor

PhD students:

- Başa Ioana Adela: Contributions on the obtain of the biodiesel
- Sălăgean Ioana Ramona: Contributions on carbohydrate based polymers synthesis and characterization
- Udrescu Valentina Liliana: Optimizing of modern ionization techniques by electrospray chip for expression determination of some glycoconjugates
- Dobren Flavius: Contribution regarding the modeling and simulation research of the co₂ dispersion process in urban environment

- Pascariu Mihai Cosmin: Tensioactive agents based on saccharide derivatives
- Paută Radu: Polymers including carbohydrates
- Chiş Ana-Maria (Pană): Saccharide derivativebased polymers
- Kiss Antonie Gabriel: Contribution regarding the polyurethans
- Mariş Ioan Dorel: *Doctoral School*
- Ştefan Liliana Marinela: Doctoral School
- 6. Prof.dr.eng. Constantin DĂESCU, PhD supervisor

PhD students:

- Pînzaru Iulia Andreea: Naphtoxidinenucleotides DNA-markers and inhibitors
- 7. Prof.dr.eng Liviu MIRCI, PhD supervisor

PhD students:

- Boran Sorina: The principle of polyfunctionality and asymmetry in the realization of new plasticizers and lubricants
- Curelea Sergiu: Polyfunctional derivatives esters for polymer processing and tribological applications
- Ismană Lidia Anița: Doctoral School
- 8. Prof.dr.eng Francisc PETER, PhD supervisor

PhD students:

- Ungureanu Mihaela: Bioethanol from lignocellulosic sources
- Ursoiu Anca: Optically active compounds obtained by enzymatic catalysis

PhD THESIS SUSTAINED

- 1. Grad Maria Elena: Synthesis of some nonbenzidinic colorants; February 2009; PhD supervisor: Prof. Dr. Eng. Lupea Alfa Xenia
- 2. Zarcula (Paul) Ana Cristina: *Biocatalitic Transformations Using Immobilized Hydrolytic Enzymes by the Sol-Gel Methods*; April 2009; PhD supervisor: Prof. Dr. Csunderlik Carol

PUBLICATIONS

BOOKS

- Hădărugă, D. I., *Compuşi odoranți-aromatizanți naturali şi de sinteză*, Ed. ArtPress, Timişoara, 2009, ISBN 978-973-108-185-4 (published in Romanian)
- Zarcula Ana Cristina, *Reactii biocatalitice* mediate de enzime hidrolitice imobilizate prin metoda sol-gel, Ed. Politehnica, Timisoara, 2009, ISBN 978-973-625-866-4 (published in Romanian)
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PUBLISHED PAPERS

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- I. M. C. Ienascu, A. X. Lupea, I. M. Popescu, M.A.Padure, A.D.Zamfir, The synthesis and characterization of some novel 5-chloro-2-(substituted alkoxy) – N - phenylbenzamide derivatives, *Journal of Serbian Chemical Society* 2009, 74(8-9), pp. 847-855, ISSN 0352-5139
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19-24 July, 2009, Luxemburg 2009, Book of Abstracts, 252, 1

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