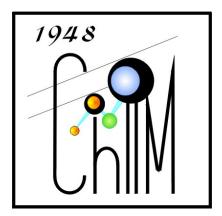
FACULTY OF INDUSTRIAL CHEMISTRY AND ENVIRONMENTAL ENGINEERING



Pta. Victoriei, nr. 2 300006-Timişoara, Romania Tel: +40-256-403063 Fax: +40-256-403060

E-mail: Web: secretar.sef@chim.upt.ro www.chim.upt.ro

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 approved by CNCSIS in 11.05.2001, according to CNCSIS certificate nr. 89/CC-C. The director of the Center is **Assoc. 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 characterisation of the substances
- Studies and projects for thermo-technical installations of the silicates industry
- Electrochemical processes
- Obtaining and characterization of oxide compounds

CONTACT

Faculty of Industrial Chemistry and Environmental Engineering

Department of Applied Chemistry and Engineering of Inorganic Compounds and Environmental

2, Victoriei Square

RO-300006 Timişoara

Tel: +40-256-403063

Fax: +40-256-403060

E-mail: <u>petru.negrea@chim.upt.ro</u>

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 characterisation of some oxide compounds

Keywords: solid-state, oxide compounds, unconventional methods

Organic Electrochemistry

Keywords: organic electro synthesis, organic electro reduction and oxidation

Electrocatalysis

Keywords: skeleton electrodes, thermal arc spraying, potentiometric sensors

> Electroplating

Keywords: copper, zinc, nickel electrodeposition, 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

Semiconducting 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 thermoresistant pigments

Keywords: ceramic glazes, thermoresistant 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, Cocheci Laura, Moșoarcă Giannin, Podariu Camelia, Corb Ioana, Proca Cristina, Haiduc Corina

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

Aurel Iovi, Petru Negrea, Georgeta Burtică, Rodica Pode, Laura Cocheci, Lavinia Teuca

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.

RESEARCH TEAM

Delia Perju, Marcel Suta, Carmen Rusnac, Raul Moldovan, Doru Dumitrel

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

Delia Perju, Marcel Suta, Carmen Rusnac, Doru Dumitrel, Adina Căta, Harieta Pîrlea, Raul Moldovan, Mirela Calisevici, Mirel Glevitzky, Sorin Marinescu

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.

RESEARCH TEAM

Delia Perju, Dana Silaghi – Perju, Carmen Rusnac, Gabriela Alina Brusturean, Harieta Pîrlea, Sorin Marinescu

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.

RESEARCH TEAM

Delia Perju, Dana Silaghi Perju, Carmen Rusnac, Gabriela Alina Brusturean, Harieta Pîrlea, Sorin Marinescu

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 absorption-desorption with chemical reaction processes.

RESEARCH TEAM

Teodor Todinca, Carmen Rusnac, Alina Brusturean, Cristian Tanasie, Adina Cata

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

Zeno Gropsian, Andra Tamas

Researches in PERFORMANCE OF COLUMNS WITH STRUCTURED PACKINGS

The structured packings present a high efficiency by comparison with the random packings 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

Zeno Gropsian, Andra Tamas, Nadia Pop

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 Ștăfnescu, Marcela Stoia, Raluca Dumitru, Ilie Julean, Mihail Bîrzescu

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, Zoltan Ecsedi, 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 quinone, hydroquinone, ethylene glycol have been analyzed, especially in undivided electrochemical reactors. Studies upon mediated reduction and oxidation of organic compounds have been undertaken.

RESEARCH TEAM

Maria Nemeş, Nicolae Vaszilcsin, Andrea Kellenberger, Mircea Dan, Narcis Duțeanu

Researches in *ELECTROCATALYSIS*

Obtaining, characterization and application of 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

Maria Nemeş, Nicolae Vaszilcsin, Andrea Kellenberger, Mircea Dan, Narcis Duțeanu, Cristina Petrescu

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, Maria Nemeş, Andrea Kellenberger, Mircea Dan, Narcis Duțeanu, Cristina Petrescu, 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 -O₂ 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, Maria Nemeş, Andrea Kellenberger, Mircea Dan, Narcis Duţeanu, 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: SiO_2 - R_2O , P_2O_5 - R_2O and B_2O_3 - R_2O .

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 Ti^{4+} 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 glasssupport 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, Zoltan Ecsedi, 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. CNCSIS Grant No 27688/14.03.2005, theme 32, code 531, type A: *Methanol – air fuel cells with skeleton nickel electrodes obtained by thermal arc spraying*

Value: 10,000 RON

Director: Assoc.prof.dr.eng. Nicolae VASZILCSIN

Members:Prof. dr. eng. Corneliu DAVIDESCU
Assoc. prof. dr. eng. Maria NEMEŞ
Lect.dr. Mircea Niculescu
Assist.eng.Andreea KELLENBEGER
PhD student Mircea DAN
PhD student Narcis DUŢEANU
Dr. eng. Nicoleta PLEŞU

FIELD DESCRIPTION: Non-polluting energy sources, nanotechnologies.

ACTIVITIES AND RESULTS:

Study of the electrode processes on skeleton nickel based electrodes in alcaline media and the conception of a methanol-air fuel cell.

2. CNCSIS Grant No. 27688/14.03.2005, theme 3, code 536, type A: Implementation of ecological production and ecodesign in drinking water treatment technologies

Value: 47,900 RON

Director: Prof. dr.eng. Georgeta BURTICA

Members: Prof. dr. eng. Aurel IOVI Prof. dr. Eveline POPOVICI Assoc. prof. dr. eng. Rodica PODE Assoc. prof. dr. eng. Petru NEGREA Lecturer dr. eng. Ioan URSOIU Lecturer dr. eng. Adina NEGREA Lecturer eng. Eugen LUNGU Assist. eng. Florica MANEA Assist. eng. Marius GHEJU Assist. eng. Giannin MOSOARCA Assist. eng. Laura Cocheci, PhD student Corina Orha

FIELD DESCRIPTION: New technologies of drinking water

ACTIVITIES AND RESULTS:

The main objective referred on water quality control, i.e. halogenated organics (TOCl, THM) and their removal from water.

3. CNCSIS Grant No. 27688/14.03.2005, theme 19, code 535, type A: *Recovery and reuse technology of metallic ions from industrial waste for minimization pollution*

Value: 9,000 RON

Director: Assoc. prof. dr. eng. Petru NEGREA

Members: Prof. dr. eng. Aurel IOVI

Prof. dr. eng. Georgeta BURTICA Assoc. prof. dr. eng. Rodica PODE Lecturer dr. eng. Adina NEGREA Lecturer dr. eng. Ioan URSOIU Assist. eng. Eugen LUNGU Assist. eng. Angela MAGDA Researcher CPI dr. eng. Corina IOVI Assist. eng. Marius GHEJU Assist. eng. Florica MANEA Resch. CP II eng. Cornel BOGATU Resch. CP III eng. Dan ROSU Resch. CP III eng. Monica IHOS Resch.CPII dr.eng. Dimitrie BOTAU Assist. eng. Laura COCHECI PhD student Mihaela ZAPARTAN PhD student Lavinia TEUCA Student Ileana Radu

FIELD DESCRIPTION:

EU directives environmental pollution reduction, technology changes and reduction of matters and energy consumption.

ACTIVITIES:

The aim of the project is the recovery and reusing of metallic ions from industrial wastes. At the beginning, the theoretical studies concerning metallic ions analysis and recovery possibilities were studied. The chemical composition of wastewaters and residual solutions (e.g.: Cu, Zn, Ni, Cr, Fe, Mn, Cd, Pb, Hg) provided by real technological processes were established; soil pollution control with heavy metals (e.g.:Cu, Zn, Fe, Mn, Cr, Mo, Ag), especially for zone with high risk; metal analysis from industrial wastes (slag, ashes, chip, PAFS, sludge and filtration sludge); extraction and capitalisation processes were tested.

4. CNCSIS Grant No. 27688/14.03.2005, theme 21, Code 714, type A: New Synthesis Methods for Controlled Properties Nanomaterials

Value:	11,000 RON		
Director:	Prof.dr.eng. Cornelia Pacurariu		
Members:	Prof.dr.eng. Dumitru Becherescu		
	Prof.dr.eng. Ioan Lazău		
	Prof.dr.eng. Corneliu Davidescu		
	Lect. dr. eng. Cornelia Muntean		
	Lect. dr. Mircea Niculescu		
	Lect. dr. eng. Romul Marius Jurca		
	Assist. eng. Radu Lazau		
	Prep. eng. Radu Ardelean		
Eng. Irina Parascanu			
	PhD student eng. Robert Ianoş		
	Student Octavian Matea		
	Student Cristina Stanila		

FIELD DESCRIPTION:

A new synthesis method based on thermal conversion of some heterpolynuclear complex combinations resulted by 1,2-ethandiol oxidation with metallic nitrates.

ACTIVITIES AND RESULTS

Synthesis of complex combinations by 1,2ethandiol oxidation with La, Al and Cr nitrates in the desired ratio; thermal treatment of the complex combinations obtained at 800, 900, 1000, 1100, 1200°C; phase compozition evolution and cristallites size assessment by X-Ray diffraction

5. CNCSIS Grant No. 27688/14.03.2005, theme 29, Code 648, type A: $Ni_XZn_{(1-x)}Fe_2O_4$ nanocomposites with controlled magnetic properties, obtained through two unconventional, original synthesis methods

Value:	15,000 RON
Director:	Assoc.prof.dr. Mircea Ştefănescu
Members:	Prof.dr.eng. Ilie Julean
	Prof.dr. Ioan Hrianca
	Lect. dr. Mihail Bîrzescu
	Lect. dr. eng. Cornelia Muntean
	Lect. dr. Costică Caizer
	Lect. Paul Barvinschi
	Assist. eng. Marcela Stoia
	Assist. eng. Erika Reisz
	Assist. eng. Liviu Costea
	PhD student eng. Thomas Dippong
	Eng. Renate Murgan
	Student Oana Stefănescu

FIELD DESCRIPTION

Synthesis through unconventional methods of nanocomposites with controlled magnetic and optic properties and their characterization

ACTIVITIES AND RESULTS

Determination of the optimal conditions for the synthesis of Ni-Zn ferrite nanoparticles through the thermal decomposition of heteropolynuclear complex combination of glyoxilate type; characterization of the nanoferrite through thermal RX diffractometry, magnetic analysis, measurements; determination of the optimal

conditions for the synthesis of Ni-Zn ferrite nanoparticles embedded in silica matrix, through a modified sol-gel method; characterization of the ferrite forerunners and of the nanocomposites (Ni,Zn)Fe₂O₄ formed in silica matrix through thermal analysis, RX diffractometry, magnetic measurements; study of the magnetic properties (saturation magnetization, magnetic susceptibility) of the synthesized nanocomposites and the correlation between magnetic properties and the composition and particle dimension of the nanoferrite.

6. CNCSIS reserch grant, NO. 26788/2005, theme 23/2005, code CNCSIS 625, type A – Simulation and optimum operation with advanced processes control systems for research plants from chemical industry

Value: 20,000 RON

Director: Prof.dr.eng. Delia Perju

Members: Assoc.prof.dr.eng. Marcel Şuta Assoc.prof..dr.eng. Dana Silaghi-Perju Lect.dr.eng. Carmen Rusnac Assist.dr. Gabriela-Alina Brusturean PhD student eng. Doru Dumitrel PhD student eng. Adina Căta PhD student chem-fiz. Harieta Pîrlea PhD student eng. Raul Moldovan

FIELD DESCRIPTION

Elaboration, design and realization of a reference prediction model for very small gas and liquid flows.

ACTIVITIES

Design and realization of a reference model.

7. CNCSIS Project, Type: A, Code: 208, Contr. No: 27688/14.03.2005, Strategies Regarding the Implementation of Some Ecotechnologies for Pollution Removal High Polluted and Ecological Critical Soils

Value: 4,000 RON

- Director: Assoc. prof.dr.eng. Vasile PODE
- Members: Prof. dr. chim. Eveline POPOVICI Prof. dr. eng. Rodica PODE Assist. dr. eng. Florica MANEA Assist. eng. Laura COCHECI PhD student Corina MACARIE

FIELD DESCRIPTION

The project tasks are referring to both important aspects of scientific knowledge and also to sustainable development. To realize a sustainable development, the removal of negative actions which are responsible for degradation of natural resources and environmental quality is necessary. The research tasks within the framework of the objective based on the setting up of means, tools and procedures for risk assessment and natural, antropic impact on socio-ecological complexes from Romania territory (west country side) reach the following subjects: natural and antropic hazard, protection systems, rehabilitation and reconstruction (special for high polluted soils).

ACTIVITIES

- Studies regarding the synthesis of a new adsorbent material consisting of magnetite onto zeolitic support. The adsorbent material could be used for pollution abatement in viscous media contaminated by highly toxic metal ions, which could be separated afterwards based on their magnetic properties.
- Establishing the relationships between synthesis conditions and magnetic properties of the new adsorbent with magnetic properties based on natural zeolite.
- Studies regarding the recovery of heavy metals from polluted soils.
- 8. CNCSIS Grant No. 27688/14.03.2005, theme 2, Code 42, type Td: Turning into good of the tanned leather wastes from the leather industry in obtaining thermoresistant pigments with Cr (III) content

Value: 8,000 RON Director: Eng. Radu-Ioan Lazău

FIELD DESCRIPTION

The tanned leather wastes from the leather industry have been successfully used as chromium source in the raw materials mixtures designed to obtain thermoresistant pigments with chromium content for the ceramic industry. The specific features of the synthesis assimilates this to the combustion method, newly mentioned in the literature as an unconventional synthesis method.

ACTIVITIES

Assessment of the chromium content of the leather wastes; synthesis of thermoresistant pigments with different crystalline structures: i) spinel; ii) tin sphene; iii) perowskite; testing of the obtained pigments in faience glazes.

- 9. CEEX PROAQUA 631/03.10.2005: Innovative and durable technologies furtherance for drinking water treatment
- *Value:* 271,000 RON
- Director: Prof. dr.eng. Georgeta Burtica
- Members:Prof. dr. eng. Corneliu Davidescu
Prof. dr. eng. Aurel Iovi
Prof. dr. eng. Rodica Pode
Assoc. prof. dr. eng. Petru Negrea
Lecturer dr. eng. Ioan Ursoiu
Lecturer dr. eng. Adina Negrea
Assist. dr. eng. Florica Manea
Assist. dr. eng. Giannin Mosoarca
Assist. eng. Marius Gheju
Assist. eng. Laura Cocheci
PhD student eng. Corina Orha

PhD student eng. Cristina Proca PhD student eng. Maria Ioana Corb PhD student eng. Camelia Podaru PhD stud. eng. Dan Cristian Danielescu PhD student eng. Aniela Carmen Pop PhD student eng. Adriana Bebeselea

FIELD DESCRIPTION

The research fields are focused on new technologies of drinking water.

10. CEEX RIWA-TECH - 62/03.10.2005: Advanced wastewater treatment technologies for the recycling of industrial effluents

Value: 143,708 RON

Director:Prof. dr.eng. Georgeta BurticaMembers:Assist. dr. eng. Florica ManeaPhD student eng. Cristina Proca

FIELD DESCRIPTION

The research fields are focused on new technologies of industrial wastewater.

ACTIVITIES AND RESULTS

The main objective referred on salvage and capitalization of substances from residual effluent.

11. CEEX – CD Project no. 5599/2005: Multifunctional porous oxidic materials for removal and degradation of priority dangerous substances from waters

Value: 30,000 RON

Director: Prof.dr.eng. Rodica Pode *Members:* Assist.eng. Laura Cocheci

FIELD DESCRIPTION

Researches related to synthesis and certain post – synthesis treatments of the new micro – and mesoporous oxidic materials, with high efficiency in the retaining processes of the main priority dangerous pollutants from waters.

Synthesis of new multifunctional synthetic porous oxidic materials, with the same functionality as international ones

Studies concerning the water remediation by decreasing of the inorganic and organic load

ACTIVITIES

Literature research concerning the national and European legislation on the pollution determined by certain dangerous substances discharged into the aquatic environment.

12. CEEX – CD Project no. 59/2005: Biotechnologies integrated with physico – chemical processes for the municipal wastewaters and the sewage sludge treatment in order to water recycling and sludge capitalisation or/and discharge into environment

Value:	27,500 RON
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Director: Prof.dr.eng. Rodica Pode

Members: Assoc.prof.dr.eng. Petru Negrea Assist.eng. Laura Cocheci Assist.eng. Marius Gheju

FIELD DESCRIPTION

Development of the innovative biotechnologies integrated with physico – chemical processes for the advanced treatment of the municipal effluents in order to recycling.

Development of the technologies for the sewage sludge treatment with the aim of agricultural, industrial and peisagistical reusing or ecological final deposition

ACTIVITIES

Complex technical analysis regarding municipal wastewaters and sludge treatment processes (efficiency, quality, demands) accordind the European and national reglementation

- 13. CEEX reserch grant, PII, No. 057/03.10.2005 – Soil exoneration using intensive methods from radioactive minerals exploitation and processing areas in the condition of naturals disasters or entropic accidents, acronim RESOLRAD
- *Value:* 3,000 RON

Director: Prof.dr.eng. Delia Perju

Members: Assoc.prof.dr.eng. Dana Silaghi-Perju Lecturer dr eng. Carmen Rusnac Assist.dr. Gabriela-Alina Brusturean PhD student chem-phys. Harieta Pîrlea

FIELD DESCRIPTION

Studies regarding chemical decontamination of soil in presence of ultra-sounds.

ACTIVITIES

Mathematical modeling and methods regarding the transfer mechanism in solid-liquid heterogeneous systems in order to establish the optimal hydrodynamic parameters

Implementation of interface equipments in measurement devices

14. CEEX Research grant: 36-CEEX-103/10/10/2005, Modern technology for ecological fuel ethers synthesis - TEMOSIE

Value: 5,000 RON

Director: Prof.dr.eng. Teodor TODINCA

Members: Lect. dr. eng. Carmen RUSNAC Assist.dr. Gabriela-Alina Brusturean

FIELD DESCRIPTION: Technology and catalysts for fuel ethers synthesis (TAME, ETBE, etc.).

ACTIVITIES

Intrinsic kinetics studies on the ethers synthesis: literature review and pilot plant design.

- 15. CEEX-Module II Research project of Human Resources for Research; Project type of Excellence Research for young researches (ET), Smart sensors for wastewater quality monitoring
- Value: 20,000 RON

Director: Assist.dr.eng. Florica MANEA

Members: PhD student eng. Maria Ioana Corb PhD student eng. Cristina Proca PhD student Andreea Ciorba

FIELD DESCRIPTION

This research proposal addresses the urgent needs for providing enhanced timely monitoring of organic pollutants in wastewater streams through the development of a chemical sensor based on an array of copper-copper oxides.

The individual miniaturized sensors and the smart sensors with different geometries will be manufactured, using mechanic and lithographic techniques. The following device parameters, i.e., sensitivity, selectivity, detection limits, stability, and short response time will be studied in detail. In addition, issues related to disposable, re-usable, and renewable smart sensors are being addressed in this research project.

While this novel type of smart sensors is focused on innovative routes of monitoring important pollutants in wastewater streams, the research goal is to contribute to the achievement of a major impact on the protection of the quality of water and the removal of impurities.

 CEEX Project: PC-D04-PT04-259/2005, 2005-2007, Obtaining of TiO₂ nanocrystal doped with metal ions through alternative methods. Study of their applications in health, biology and environmental fields.

Value: 1,130,500 RON

Director: Assoc.prof.dr. Mircea Ştefănescu Members: Prof.dr.eng. Lucian Mircea Rusnac Assist. eng. Marcela Stoia

FIELD DESCRIPTION

Nanoscience and nanotechnologies; obtaining of new nanomaterials (TiO_2 nanocrystals doped with metal ions) with controlled properties trough new technologies and study of their applications in different fields: health, biology, environmental.

ACTIVITIES AND RESULTS

Studies on the sol-gel synthesis of TiO_2 nanocrystals doped with metallic ions; studies on the microwave or sonochemical assisted hydrothermal synthesis of TiO_2 nanocrystals doped with metal ions; investigations on the fotocatalytic and bacillicide properties of the TiO_2 nanocrystals doped with metal ions; physico-chemical characterization of synthesized TiO_2 nanoparticles (BET, SEM, TEM, RX difractometry); comparative study of the properties of TiO_2 nanocrystals synthesized through different methods.

17. CEEX – CERES Program, CEx05-D11-38/06.10.2005, Advanced structural materials for optoelectronics micro-systems

Value: 6,363 RON Director: Lect.dr.eng. Adina Lația Members: Lect.eng. Cosmin Vancea

FIELD DESCRIPTION

Advanced materials and technologies

 Romanian - Hungarian bilateral scientific research Project RO-20/2002 – 2005, Institute of Physics and Laser Spectroscopy, University of Pecs

Responsible of the Romanian research team: Prof.dr.eng. Georgeta Burtica

Members:Assist.dr.eng. Florica ManeaPhD student eng. Corina OrhaPhD student eng. Cristina ProcaPhD student eng. Maria Ioana CorbPhD student eng. Camelia PodaruPhD student eng. Dan Cristian DanielescuPhD student eng. Aniela Carmen PopPhD student eng. Adriana Bebeselea

ACTIVITIES AND RESULTS: Research trainings for PhD students. Laser Spectroscopy for structural inorganic materials analysis.

PhD RESEARCH ACTIVITIES

1. Prof. dr. eng. Ilie JULEAN, PhD supervisor in *Chemistry*

PhD students:

- Barbul Lucian: Homo- and heteropolynuclear compounds with hydroxycarboxylic acid anions as ligands, used as precursors for oxidic systems
- Marian Eleonora: Complexes of transition elements with medicinal substances
- Stoia Marcela: Studies concerning the influences that affect the stability of some complexes with applications in analytical chemistry
- Ursulescu Georgeta: Studies concerning the accuracy and precision of some analysis techniques of biological materials
- Bota Marcela: Studies concerning some basic compounds used to obtain inorganic pigments
- Dippong Thomas: Investigations about the compounds obtained through complexing or precipitation reactions with transition metal ions
- Ilici Maria: Studies about complexes of transition metals with heterocyclic compounds

2. Prof. dr. eng. Aurel IOVI, PhD supervisor in *Chemical Engineering*

PhD students:

- Bel Gabriela: Studies regarding the waters purification from nitrite inorganic compounds
- Albulescu Gabriela: Studies about the obtaining process of nitro phosphates complexes fertilizers with microelements
- Berbecea Adina: Studies about the obtaining process of complex fertilizers based on ammonium phosphates with microelements
- Popescu Elena Laura: Studies about the obtaining process of the complex combinations of the metals ions with spectral use
- Lungu Eugen: The use of activated oxidants in the waters treatment domain
- Morgovan Claudia: The reuse of the metals ions from galvanic industry wastes under fertilizers with microelements
- Marşavina Dalila: The studies of the equilibriums from the undergrounds waters in the view of the use of these as drinkable waters
- Roşu Dan: The behavior of the complex combinations with microelements in the obtaining process of the fertilizers
- Zapârţan Elvira Mihaela: Studies regarding the obtaining of the complex fertilizers with high content of active substances
- Magda Angela: Studies about some oxygenate compounds of boron with applied in fertilizers technologies with microelements
- Sbeşan Mioara: The characterizations of the geothermal waters and the depose monitoring what could appear in the case of their use
- Briea Carmen Doina: The engineering and quality management in the complex fertilizers industry
- Gliga Mihaela: Technologies of reuse of some useful substances from wastes
- Ihoş Monica: Unconventional technologies of elimination from water of some specific pollutants
- Gheju Marius: Specific processes of chrome elimination from waters
- Bogatu Cornel: Specific technologies in the water technology
- Ursulescu Marius: Contributions to the improvements of the corrosion resistance and of the others qualities of the metallic surfaces by cover with inorganic compounds
- Haiduc Corina Ileana: New composite materials used in water treatment
- Teuca Lavinia Afrodita: Studies about the inhibition processes of the corrosion in the refrigeration systems
- Cocheci Laura: Oxidative chemical processes for soil decontamination
- Micu Daniela: The study of the toxic compounds elimination processes from rural waters sources

- Rus Adrian Gheorghe: The study of the obtaining processes of the active principles from medicinal plants and their characterizations
- Cîrstoiu Alina Lucia: Studies about the reduction processes of the volatile organic compounds concentration from residual waters
- Andoni Mihaela: Studies about the reduction processes of the environmental pollution from mercuric compounds
- Lazău Carmen: Studies regarding the characterizations and the use of some nano materials of type TiO₂ in the ambient environmental decontamination
- Macarie Ioan: Contribution to the synthesis of some amino – organic – phosphoric with biological applied
- Rus Valeria: Studies regarding the sludge treatment from the local purification plant in the view of put in good use or elimination
- Maria Mihaela: Studies regarding the control and effect of the exposure to hard metals in the professional and unprofessional medium
- Popa Florina: Contributions to the obtaining and use of antiseptic agents based on synergetic mixture
- 3. Prof. dr. eng. Delia PERJU, Ph.D supervisor *PhD students*:
- Doru Dumitrel: Contributions to the Improvement of pH Regulating Systems
- Căta Adina: Modelling, Simulation and Optimal Process Control of Technological Processes from Food Industry
- Harieta Pîrlea: Contibution to the simulation and modeling of chemical processis for reduction of nitrogen dioxide emmissions
- Raul Moldovan: Improvement of the Heat Boundary Layer Flowmeter Performances Using Analogue-Numerical Systems
- Calisevici Mirela: Quality Performances Improvement of a Food Process Line Using Advanced Optimal Process Control
- Glevitzky Mirel: Contributions to the Quality Performances Improvement of Fruit Juices by Application of Optimization and Control Process Techniques in the Technological Installations
- Marinescu Sorin: Contributions to the Optimization Possibilities of a Waste Incineration Plant
- Bragea Mihaela Gladiola: Contributions to the Modelling and Simulation Phenomenon of Radioelements Migration in the Environment from The Uranium Industry Waste
- Dancea Daniel: Contributions to the Modelling, Simulation and Optimal Process Control of Heat Transfer Processes
- Muşuroi Luci: Contributions to the Performance Improvement of Low Pressure Equipments System

- 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 Electrothermal Gas Flowmeter 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
- 4. Prof. dr. eng. Zeno GROPŞIAN, PhD supervisor
 - PhD students:
- Bors Nicu: The investigation os 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
- Iorga Mirela: Contributions to the mass transfer intensification in electrochemical recovery of metallic ions from solutions
- Pop Nadia: Advanced methods for gases purification
- Rujan Dan: Fractals applications on describe and modelling of crystalline surfaces
- Prof. dr. eng. Georgeta BURTIĂ, PhD supervisor in Chemical Engineering PhD students:
- Macarie Amalia Corina: Contributions at the eco-technologies elaboration for the metallic ions recovery from the used electrolyte
- Furdui Petre Vili: Studies regarding the monitoring and characterization of the drinking water resources from the Romania's west region
- Jurj Nicoleta Luminita: 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

- Puiulet Mihaela: Studies concerning the removal of the iron and manganese from underground -water in view to improvement the drinking water quality
- Ramona Mihaela Ghiga: Capitalization technologies of some useful substances from wastes
- Corina Haiduc: New composite materials used in water treatment
- Cristina Proca: Water decontamination technologies used new composite materials based on innorganic salts
- Camelia Podaru: Studies about obtaining chemically modified materials with an aplication in water quality cleaning and monitoring
- Ioana Maria Corb: Studies regarding the production and the characterization of new alumina silicate materials with utilization in ecotechnologies
- 6. Prof. dr. eng. Dumitru BECHERESCU, PhD supervisor in *Materials' Science and Engineering PhD students*:
- Bartiş Tihamer: New thermoresistant pigments and their behavior in glazes and ceramic colorants
- Calapod Adriana: Concrete as an immobilization factor for some polluting materials
- Tațian Călin: Re-use of some furnace slags as construction materials
- Lazău Radu-Ioan: Study upon the parameters that influence the color of the ceramic glazes with transitional cations
- Lupa Marius: Study of the milling process with a view of its optimization
- Neamţu Ion: Re-use of the wastes from the paper industry
- Ziman Nicolae: Contributions in table ware faience technology concerning the quality and costs
- Prof. dr. eng. Ioan LAZĂU, PhD supervisor in Materials' Science and Engineering PhD students:
- Zoltán Ecsedi: Using the unconventional methods in tailored-properties oxide materials synthesis
- Alexandru Orban: Technological parameters optimization for obtaining super-aluminous products
- Robert Ianoş: enroled in 2005
- Prof. dr. eng. Nicolae VASZILCSIN, PhD supervisor in *Chemical Engineering PhD students*:
- Dan Mircea: The metal extraction from residual water in electrochemical reaction with vibrating electrodes

- > Duţeanu Narcis: Contributions on the realization pf $H_2 O_2$ fuel cells equipped with skeleton Ni electrodes and anion exchange membranes
- Petrescu Elena Cristina: Deposition of electroactive films by the sol-gel method
- Bănică Radu Nicolae: Solar cells based on CuInS₂

PhD THESIS SUSTAINED

- 1. Katalin Bodor: *Contribution to improving quality indicators of drinking water by using new reagents and technologies*, PhD supervisor: Prof.dr.eng. Delia Perju
- 2. Diana Chiş: Contributions about usage of chlorinate compounds (chlorine dioxide and chlorine) at the treatement of surface waters in drinkable objective, for improving the quality of this, PhD supervisor: Prof.dr.eng. Delia Perju
- 3. Dan Cristian Tănasie: Contribution to the modelling and numerical simulation of the gasliquid reactors, PhD supervisor: Prof.dr.ing. Delia Perju
- 4. Romance Tamara: Studies about geothermal water corrosive action from Bihor area to the exploitation, transport and used, PhD supervisor: Prof. dr.eng Aural Iovi.

PUBLICATIONS

BOOKS

- 1. Burtică, G., Negrea, A., Micu, D., Orha, C., *The Pollutants and the Environment*, Politehnica Publishing House, Timişoara, 2005, ISBN 973-625-262-0, 273 pages (published in Romanian)
- Perju, D., Şuta, M., Rusnac, C., Brusturean, G.A., Automation of chemical process – Aplications, Politehnica Publishing House, Timişoara, 2005, ISBN 973-625-217-5, 973-625-222-1, vol. I, 163 pages
- 3. Perju, D., Rusnac, C., Department of the Chemistry engineering monography, Politehnica Publishing House, Timişoara, 2005, ISBN 973-625-209-4, 61 pages
- Minea R., Tamas A., *Applications on Mass Transfer*, West Publishing House, Timisoara, 2005, ISBN 973-36-0409-7, 159 pages (published in Romanian)

PUBLISHED PAPERS

 Rădulescu, H., Micu, M., Burtică, G., Food as a potential source of consumer's nitric stress, Central European Journal of Occupational and Environmental Medicine, 11 (2), 2005, pp. 87-92

- Orha, C., Barvinschi, P., Burtică, G., Structural characterization of silver modified clinoptilolite used in water treatment, Sustainability for Humanity and Environment in the Extended connection Field Science- Economy-Policy, Scientific reunion of the special program of the Alexander von Humboldt Foundation, Timisoara, ISBN 973-625-205-1, 2005, pp. 181-185
- Popovici, E., Burtică, G., Pode, R., Barvinschi, P., Hristodor, C., *Removal of some heavy metal cations from wastewater using Romanian clays*, Sustainability for Humanity and Environment in the Extended connection Field Science-Economy-Policy, Scientific reunion of the special program of the Alexander von Humboldt Foundation, Timişoara, ISBN 973-625-205-1, 2005, pp. 189-192
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- Pode, R., Vlaicu, I., Savescu, E.M., Manea, F., Morariu, M., *Conditioning and Gravitational Sedimentation of Municipal Sludge*, 12th Symposium on Analytical and Environmental Problems, Szeged, 26 September 2005, pp. 45-49
- 6. Brusturean, G.A., Carre, J., Perju, D., Bourgois, J., *Etude experimentale du traitement par venting*, Dechets, sciences et Techniques, France, March 2005, Nr.37, ISSN 0783-3454, pp. 4-12
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- Pirlea, H., Silaghi-Perju, D., Perju, D., Suta, M., Analytical and experimental mathematical models for nitrogen dioxide dispersion in the atmosphere, basis on the monitoring of 3 meteorological parameters in Timisoara, Romania, 10th Mediterranean Congress of Chemical Engineering, 15-18 November 2005, Barcelona, Spain, topic: Process Engineering, ISBN 84-88233-27-2, pp. 549

- Brusturean, G.A., Todinca, T., Perju, D., Carre, J., Dumitrel, D., Mathematical modeling of soil venting depollution process, 10th Mediterranean Congress of Chemical Engineering, 15-18 November 2005, Barcelona, Spain, topic: Environmental Technology, ISBN 84-88233-27-2, pp. 282
- Perju, D., Şuta, M., Pîrlea, H., Moldovan, R.C., Possibilities for Constructing and Using an Electrothermal Gas Micro-flowmetter with Digital Displaying, Microcad 2005 International Scientific Conference, University of Miskolc, Hungary, 10-11 March 2005, topic: Fluid and Heat Engineering, ISBN 963-661-646-9-ö, ISBN 963-661-652-3, pp. 101-106
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- Pode, V., Rus, A., Obtaining of active components from cinnamon oil, Chim. Rev., 56, nr. 3, 2005, ISSN 0034-7752, pp.309-312
- 19. Pode, R., Pode, V., Use of Composite Materials Based on Magnetite and Zeolitic Support for Depollution of Heavy Metals Contaminated Soils, Chim. Rev., 56, nr. 4, 2005, ISSN 0034-7752, pp. 436-438
- 20. Todinca, T., Analysis and kinetic modeling of a non-ideal liquid reaction system, "Ovidius University Annals of Chemistry", 16, 2, 2005, ISSN 582-6724, pp. 261-264
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- Negrea, P., Teuca, L., Negrea, A., Lucaciu, M., Study about the elimination process of silver from solutions resulted from photographic industry, 12th symposium on Analytical and Environmental problems, 26 September 2005, ISBN 963-219-675-9, pp. 83-87
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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:

- New methods in organic synthesis
- Computational chemistry
- 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
- Volatile oils fractionation

CONTACT

Faculty of Industrial Chemistry and Environmental Engineering Department of Applied Chemistry and Engineering of Organic and Natural Compounds Str. Carol Telbisz, nr. 6 Timişoara, Romania

E-mail: mihai.medeleanu@chim.upt.ro

RESEARCH FIELDS

> New methods in organic synthesis

Keywords: synthesis of organic compounds, carbonic acid derivatives, heterocyclic compounds, chromatography, structure determination UV-VIS, FT-IR, MS, NMR, biocatalysis of organic reactions, asymmetric syntheses

Computational chemistry

Keywords: topology, graphs, structure-properties relationship (SAR), size and shape of molecules, van der Waals volume and surface, molecular mechanics, quantum mechanics methods in chemistry

Physical Chemistry. Chemically Active Species Grafted on Polymer-Supports

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

Synthesis and characterization of PVC plasticizers Keywords: PVC, plasticizer, lubricants

Oligomers with functional groups

Keywords: oligomer, functional group, reactive oligomers

Chemistry and technology of drugs and pesticides

Keywords: drug, pesticides, chemistry, technology, semisynthesis, agriculture

Chemistry and technology of dyestuffs, and textile auxiliaries

Keywords: dyes, dye accelerators, dispersants, textile auxiliaires

Performance of columns with structured packings

Keywords: wettability, specific surface

Researches in NEW METHODS IN ORGANIC SYNTHESIS

Synthesis of organic compounds (carbonic acid derivatives, heterocyclic compounds, 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), asymmetric syntheses and enantiomeric separations, synthesis and functionalization of heterocycles, heterocycles with potential biological activity.

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, carbonylchlorides, 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 hetrocyclic compounds, studies of biocatalytic processes in organic synthesis, asymmetric syntheses, separation methods and structure determination of organic compounds by UV-VIS, FT-IR, MS and NMR spectroscopy were also performed.

RESEARCH TEAM

Carol Csunderlik, Vasile Bercean, Peter Francisc, Milea Marius, Badea Valentin, Simon Monika, Mihai Medeleanu

Researches in COMPUTATIONAL CHEMISTRY

Computational chemistry as an application of topological, molecular mechanics and quantum mechanics models is a useful tool in molecular structure investigation and structure – properties (chemical reactivity and biological activity) analysis.

Applying these models to organic molecules, the informations derived from the structure of organic compounds are transformed into molecular descriptors (topological, sterical and quantum chemical) that are correlated with physical properties, chemical reactivity and/or biological activity. The correlation equations are used on one hand to explain the reactivity and biological activity of organic and natural compounds and on the other hand to predict physical and chemical properties.

RESEARCH TEAM

Mihai Medeleanu, Simon Monika, Peter Francisc, Vasile Bercean, Milea Marius, Badea Valentin, Carol Csunderlik

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 "hybridbiomimetic catalysts phase" 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 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

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, Lucian Rusnac, Geza Bandur, Gerlinde Grandtner, Mihaela Nechita

Researches in *CHEMISTRY AND* **TECHNOLOGY OF DRUGS AND PESTICIDES**

Synthesis, analysis and testing of total and semisynthetic 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 microproduction and industry.

RESEARCH TEAM

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

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 fibres has been studied. Syntheses of some key intermediates for organic dye technologies have also been performed.

RESEARCH TEAM

Ioan Macarie, Simona Popa

RESEARCH PROJECTS

1. CNCSIS Grant 27688/14.03.2005 (Additional papaer/2005) theme 9, code 135, type A: Bis(o-Nitrophenyl) Carbonate, a Potential Reagent in Fine Organic Synthesis Included Combinatorial Chemistry and Asymmetric Synthesis (Carbonates, Policarbonates, Carbamates, Oxazolidinones Synthesis

Value: 18,000 RON

- Director: Prof. dr. chem. Carol CSUNDERLIK
- Members: Prof. dr. eng. Mihai MEDELEANU Lect. dr. eng. Marius MILEA Assist. eng. Monika SIMON Ph.D student eng. Andreea TARTA Ph.D student eng. Adina SEGNEANU Student Maria TUROCZI

FIELD DESCRIPTION

The purpose of our studies is to find substitutes for phosgene from the carbonic acid functional derivatives, able to react efficiently with various nucleophiles for obtaining the same compounds like those resulted with phosgene and also new possible compounds. Moreover, we are interested in the study by X Ray diffraction of the nanostructures for the new compounds which are going to be obtained. In the previous studies we were focused on the reactivity of some organic carbonates like N,N'disuccinimidyl carbonate, di-2-pyridyl carbonate, N.N'-diphtalimidyl carbonate, bis(p-nitrophenyl) bis(o-nitrophenyl) carbonate and carbonate. Further, we want to synthesise some new onitrophenyl carbamates and ureas using bis(onitrophenyl) carbonate and various amines. As we have already found out from previous studies, these kind of reactions occur very fast in mild conditions. A study of intra- and inter-molecular hydrogen bonds by X Ray diffraction is going to be made for the o-nitrophenyl carbamates resulted and which may be considered as model compounds for protein structure. Then, the reaction with oxigene nucleophiles, as alcohols, phenols, bisphenols, carboxilic acids, carbohydrates and also with binucleophiles as diamines, dialcohols. aminoalcohols, aminoacids are going to be studied taking into account the advantages of this method compared to those already published. From the reactions with binucleophiles a special interest present the obtaining of some oxazolidinones with importance in asymmetric synthesis where they are used as chiral auxiliary for the alkylation of enolates or in asymmetric aldol reactions and Diels-Alder reactions. The monitorizing of the reactions will be made by FT-IR spectroscopy using special manufactured IR silica-cells. Finally, the solidsupport reactions study is going to be made by testing the carbonate efficiency in synthesis of some biological active compounds.

ACTIVITIES

In the year 2005 the activities were centered on the following investigation topics:

- The study of the reactions between bis(onitrophenyl) carbonate and various N,O- and N,N-binucleophiles by FTIR spectroscopy in order to find the optimal conditions for obtaining the desired products.
- Synthesis and characterization of some known oxazolidin-2-ones using bis(o-nitrophenyl) carbonate as carbonylation reagents
- Synthesis the new method of some chirals oxazolidin-2-ones useful in asymmetric synthesis
- Synthesis and characterization of the benzoxazolidone from bis(o-nitrophenyl) carbonate and o-aminophenole
- Synthesis and characterization of some known imidazolin-2-ones using bis(o-nitrophenyl) carbonate as carbonylation reagents
- 2. CNCSIS Project, Type: AT, Code: 25, Contr. No: 27688/14.03.2005, Bioactive nanocapsules: obtaining, characterization, molecular modeling of the cyclodextrinbiomolecule systems
- Value: 18,000 RON

Director: Lect. dr. eng. Daniel-Ioan HĂDĂRUGĂ *Members:* Lect. dr. eng. Nicoleta HĂDĂRUGĂ

PhD stud.eng. Laurențiu ORDODI

FIELD DESCRIPTION

The goal of this grant named Bioactive nanocapsules: Obtaining, characterization and modeling of cyclodextrin-biomolecule systems is the study of molecular encapsulation of odorant compounds, volatile oils, or fatty acids in α -, β -, and γ -cyclodextrin, used in medicine, pharmacy, foodstuffs, organic and analytical chemistry.

ACTIVITIES

The research presumes a first step of literature survey, used also for Natural Compounds Chemistry, Natural Drugs, Flavors and Fragrances, The Degradation and the Protection of Foodstuffs courses.

The objectives and the activities of this study are:

- The obtaining of the cyclodextrin-odorant compound, volatile oil, fatty acid inclusion complexes;
- ➤ The analysis of the complexes by thermogravimetry-TG (establishing the quantities of encapsulated biomolecule), differential scanning calorimetry-DSC (for the evaluation of the energetic effects among the heating of the complex), gas chromatography (GC-FID and GC-MS for the analysis of odorant compounds, volatile oils, and derivatized fatty acids used as guest compounds, in order to establishing the encapsulation

competitivities), liquid chromatography-HPLC (for the establishing of the type and concentration of inclusion complexes for the multicomponent systems);

- The mathematical and molecular modeling of the nanoencapsulation (using the molecular mechanics and semi empirical methods implemented in specific software) between cyclodextrins and biomolecules.
- 3. CEEX Project (Partner 1), Code: P-CD-18, Contr. No: 18/10.10.2005, Nanocomposite / nanocrystal synthesis with applications in biotechnology, agriculture, food, health, and environment (NUSA)

Value: 137,000 RON

Director: Lect. dr. eng. Daniel-Ioan HĂDĂRUGĂ

Members: Lect. dr. eng. Mirabela PĂDURE Student eng. Svetlana CACIG Eng. Tiberiu BALAZS

FIELD DESCRIPTION

this project, the obtaining of In the micro/nanoparticles and micro/nanocapsules (especially with bioactive compounds), isolation and purification of the studied biocompounds (from the Allium, Chelidonium, and Nicotiana species, especially), and the analysis and application of bioactive compounds and micro/nanoparticles and/or micro/nanocapsule will be studied. The most used encapsulation matrices are oligo- and polysaccharides, lipids, and synthetic polymers; in this project the cyclodextrins will be used as encapsulation matrice; they are composed especially by three cyclic oligosaccharides which are industrial produced: α -, β -, and γ -cyclodextrin, known as Schardinger dextrins, A/B/G-CD, C6-8A. The analysis of the micro/nanocapsules is realized by chromatographyc methods (HPLC, TLC, GC for derivatized compounds), photometry, termoanalytical methods (thermogravimetry, differential scanning calorimetry, X ray diffaction, and electronic microscopy methods (SEM, TEM).

ACTIVITIES

- Obtaining of the raw extracts by steamdistilation, extraction with organic solvents; separation of the biocompounds;
- Purification of the biocompounds: aliin, allicin, dialyl-disulfide, dialyl-trisulfide, chelidonin and related alkaloids, nicotin and related alkaloids will be attained by preparative HPLC;
- Analysis of biosystems and biocompounds: GC-FID, GC-MS, HPLC, FT-IR
- Obtaining of the nanoparticles/nanocapsules with cyclodextrins
- Analysis of nanoparticles/nanocapsules (TG, DSC, TEM, SEM)

- Applications of nanoparticles/nanocapsules in different areas (biotechnology, agriculture, food, health, environment)
- 4. CEEX Project, Postdoctoral programme PD3 2005, *Carbohydrates based new materials*

Value: 60,600 RON

Director: Prof. dr. eng. Lucian Mircea Rusnac

FIELD DESCRIPTION

The postdoctoral programme - Carbohydrates Based New Materials - is dedicated to the development of highly qualified human resources. To achieve this major objective, a scientific proposal, combining fundamental and applied researches, is made. Its subject is the synthesis and characterisation of two new types of carbohydrates based materials – drug vectors and biodegradable polymers.

ACTIVITIES

Common components, but having different functions in the new materials, are: fatty acid moieties (ensure compatibility of drug vectors with neuronal tissues and respectively internal plasticization of glycopolymers) and sugar moieties (ensure drug vectors' compatibility with the body fluids and respectively biodegradability of glycopolymers).

In the drug vectors these components are connected by new polyhydroxylic compounds synthesised by methods derivate from carbonic acid chemistry. Glycomonomers are synthesised by the attachment of one or two acrylic, methacrylic or vinylic groups to the sugar. Subsequent (photo) polymerization of these monomers forms the glycopolymers.

All the new materials will be characterised (physico-chemical and functional properties). Most of the investigation methods are available and others are obtained by co-operation with universities from France (d'Artois, Montpellier 2) and Germany (Braunschweig).

The development of highly qualified human resources involves different activities, e.g. development of literature reviewing capacity, improvement of synthesis and analysis skilful, improving of individual responsibilities and of the team-work performance. Stages abroad will also contribute to achievement of this important (for EU also) objective.

PhD RESEARCH ACTIVITIES

- 1. Prof. dr. Carol Csunderlik, PhD supervisor *PhD students:*
- Stricatu (Mahagney) Sabina: Synthesis and Characterization of Some Functionalized Polyethers with Lypophylic Hydrocarbonated Chains and with Polar Anionic Groups
- Stanoiev Zlatimir: Sythesis and Characterization of Heterocyclic Compounds

Used in Derivatization Reactions of Natural Polymer Compounds

- Kiss (Popa) Claudia: Enantioselective Synthesis Using Enzyme Catalysed Biotransformations in the Field of Functional Derivatives of Carbonic Acid
- Szöcz-Biro Emese: Synthesis of Functional Derivatives of Polyhydroxilic Compounds Using Biotransformation Reactions with Free or Immobilized Enzymes
- Tarţa (Micle) Andreea: Synthesis and Applications of Reactive Functional Derivatives of Carbonic Acid
- Segneanu Adina: The Use of Some Reactive Organic Carbonates as Protecting or Activating Reagents in Peptide Synthesis
- Pintea Beniamin-Nicolae: New Synthetic Methods for Obtaining of N-Substituted Derivatives of the Cyclic Imides of Dicarboxylic Acids
- Şofei Daniela: Contributions to the Study of Functionalization Reactions of Nitrogene Containing Heterocycles
- Susan Simona: Studies of Separation, Purrification and Applications of Some Natural Compounds Isolated from Capsicum
- Zarcula (Paul) Ana Cristina: Biocatalitic Transformations Using Immobilized Hydrolytic Enzymes by the Sol-Gel Methods
- 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
- Neanu Cristian: Synthesis and Studies of Some Modified Carbohydrates with Potential Biologic Activity
- Turoczi Cristina: Reactive Organic Functional Derivatives of Carbonic Acid
- Bosilcov Alin: Studies of Methods for Organic Synthesis in the Field of Derivatives of Essential Oils
- Palani Adil: Thermal Decomposition of N-Carbamoil Derivatives of Cyclic Imides
- 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
- Mărieş Gheorghe Radu Emil: Contributions to injection parameter's study of thermoplasts for performance sports articles
- Roşca Cristina: Interaction characterization of rubber-filling
- Mişcă Ruxanda Manuela: Researches about improvement of physico-mechanic characteristics of synthetics elastomers's compounds
- Găşpărel Ovidiu Virgil: Contributions at some elastomers wastage recovery's study

- Uscătescu Maria Ramona: Contribution at study of rubber mixture's adherence at transport band's base
- Stana Simona-Maria: Contribution at synthesis and usage study of reagent oligomers
- Grandtner Gerlinde Iuliana: Contributions at study of reagent oligomers usage in nanocomposites
- Prof. dr. eng. Alfa-Xenia Lupea, PhD supervisor PhD students:
- Cacig Svetlana: Vegetable extracts possible used as natural ingredients for drugs, cosmetics, food
- Cătănoiu Gabriela: Contributions to the synthesis and characterization of new phase transfer catalysts from quaternary ammonium salts class
- Ienaşcu Ioana Maria Carmen: Potentially biological active with o-hydroxybenzamydic structure
- Pop Mariana: Vegetable extracts, from berry, possible used in bioconstituent's oxidation processes inhibition
- Popa Ioana: Structure-properties relationships for some natural hydroxyl-quinone
- Prof. dr. eng. Corneliu DAVIDESCU, PhD supervisor in *Chemical Engineering PhD students*:
- > Ardelean Radu: *Polymer-supported catalysts*
- Peli Monica: Applications of functionalized polymers in environmental engineering
- 5. Prof. dr. eng. Lucian RUSNAC, Ph.D supervisor
- *PhD students*:Mihaela Nechita: enrolled 2005
- Başa Adela: enrolled 2005
- Sălăgean Ioana: enrolled 2005
- Dobren Flavius: enrolled 2005
- ▶ Hegheduş Mîndru Gabriel: enrolled 2005
- Prof. dr. eng. Constantin DĂESCU, Ph.D supervisor PhD students:
- Pînzaru Iulia Andreea: enrolled 2005
- Burlacu Marcela Mădălina: enrolled 2005

PhD THESIS SUSTAINED

- 1. Simon Monika: Utilization of Carbonic Acid Derivatives in Fine Organic Synthesis; July 2005; PhD supervisor: Prof. Dr. Csunderlik Carol
- Cseh Liliana: Contributions to the Synthesis of Organic Ligands for Complexes with Potential Liquid Crystal Properties; November 2005; PhD supervisor: Prof. Dr. Csunderlik Carol
- 3. Nicoleta Hadaruga, *Protection and controlled release of the bioactive componds*, 6 April 2005,

PhD supervisor: Prof. Dr. Eng. Alfa Xenia Lupea

4. Erika Reisz, Aspects regarding chemistry and photochemistry of ozone in aqueous media, PhD supervisor: Prof. Dr. Eng. Corneliu Davidescu

PUBLICATIONS

BOOKS

- Mirci L., *Thermoplastic elastomers*, Art Press Timişoara, Ed. Augusta, Timişoara, 2005, ISBN 973-7836-23-5, ISBN 973-695-160-X, 504 pages (published in Romanian)
- 2. Popa, S., Jurcau, D., Jurcau, C., Plesu, N., Organic Pigments. Vol.I. The Pigments and the Colour, Orizonturi Universitare Publishing House, Timisoara, 2005, 192 pages (published in Romanian)
- Daescu, C., *Drug Industry*, 2nd ed., Politehnica Publishing House, Timisoara, 2005, ISBN 973-625-271-X, 308 pages (published in Romanian)

PUBLISHED PAPERS

- 1. Bandur, G., Resiga, D., Pode, V., *Aspects of rheological behaviour of o-sec-butil phenoxiacetic acid esters*, Rev. Mat. Plast., 42, nr.3, 2005, ISSN 0025-5289, pp. 220-225
- Mirci, L., Boran, S., Luca, P., Boiangiu, V., New mixed esters with a complex alkyl-aryl structure considered as tribological fluids, J. Synth. Lubrication, vol.22, 2005, ISSN 0265-6582 (in press)
- Mirci, L., Boran, S., New Polymer Processing Aids of the Phtalic Class, Rev. Mat. Plast. vol. 42, Nr. 1, 2005, ISSN 0025-5289, pp. 47-59
- Mirci, L., Boran, S., Polyfunctional Plasticizers and Lubricants of Sebacic Type, Rev. Mat. Plast. vol. 42, Nr. 2, 2005, ISSN 0025-5289, pp. 124-132
- Simon, M., Csunderlik, C., Cotarcă, L., Căproiu, M.T., Neda, I., Turoczi, M.C., Volpicelli, R., Synthesis of new active onitrophenyl carbamates, Synth. Commun., 35(11), 2005, ISSN 0039-7911, pp. 1471-1479
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