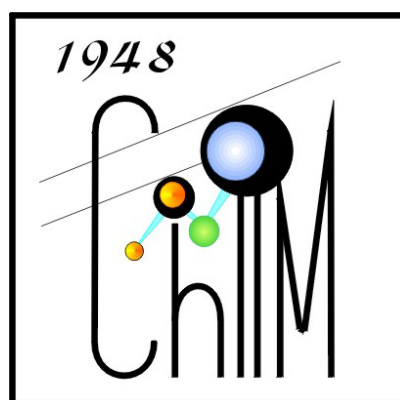


# ***FACULTY OF INDUSTRIAL CHEMISTRY AND ENVIRONMENTAL ENGINEERING***



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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 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
- Modeling, simulation and process control
- 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
- **Modeling, simulation and processes control**  
*Keywords:* simulation, control processes, modeling, fuzzy
- **Coordinative compounds analogous to the Reinecke**

*Keywords:* Reinecke salt, coordinative compounds, organic bases with nitrogen

- **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, fuel cells

- **Electroplating**

*Keywords:* copper, zinc, nickel electrode position, brighteners

- **Fuel Cells**

*Keywords:* skeleton electrodes, proton exchanges, membrane

- **Synthesis of ceramic raw materials through hydrosilicatic forerunners**

*Keywords:* ceramic, hydrosilicatic, synthesis

- **Studies and projects for thermo-technical installations of the silicates industry**

*Keywords:* silicates industry, thermo-technical installations

- **Research upon refractory and high temperature heating insulation materials**

*Keywords:* high temperature, heating, insulation materials

- **Fast ion-conducting glasses. Redox equilibrium in glasses. Investigations upon new vitreous systems**

*Keywords:* conducting, glasses, redox equilibrium, vitreous systems

- **Studies upon the manufacturing of some mullite - cordierite and high alumina technical ceramics**

*Keywords:* mullite, cordierite, alumina, ceramics

- **Studies and researches in chemistry and technology of cements with low firing temperatures**

*Keywords:* cements, firing temperature

- **Studies and projects for thermo-technical installations of the silicates industry**

*Keywords:* thermo-technical installations, silicates industry

#### **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, Camelia Podariu, Ioana Corb, Cristina Proca, Corina Haiduc

#### **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, Alina Cîrstoiu

#### **Researches in MODELING, SIMULATION AND CONTROL OF ABSORPTION - DESORPTION PROCESSES**

Modeling, simulation and control of absorption-desorption with chemical reaction processes. Steady-state (including composition and phase's temperature modification through height) and unsteady-state process simulation.

Numerical process simulator; tests for new gas-liquid, tower pickings.

#### **RESEARCH TEAM**

Teodor Todinca, Romulus Minea, Lazăr Gabor

#### **Researches in EQUIPMENT FOR RESEARCHING PLANTS AND PILOTS AUTOMATION IN CHEMICAL INDUSTRY**

Some specific equipments of automating for research plants from chemical industry (measurement and automat regulation of small and micro gas and liquid flows, gas and liquids compositions, pressure) using like information support low pressure signals in 500-3000 N/m<sup>2</sup> domain.

Elaboration, projecting and realization of reference models for a system of low pneumatic elements with high function performances.

#### **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, Adina Căta, Mirela Calisevici, Mirel Glevitzky

#### **Researches in NEURAL NETWORKS APPLIED IN CHEMISTRY AND CHEMICAL ENGINEERING**

Using Neural Networks in Process control, Modeling and Simulation of Chemical Processes and studies about Quantitative Structure-Properties Relationships.

Modeling and simulation of chemical processes, QSPR studies, numerical control based on Neural Networks.

#### **RESEARCH TEAM**

Delia Perju, Gabriela Alina Brusturean, Harieta Pîrlea

#### **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, Gabriela Alina Brusturean, Carmen Rusnac, Harieta Pîrlea, Sorin Marinescu.

#### **Researches in HEAT TRANSFER AT BOILING SOLUTIONS AND PROCESS INTENSIFICATION**

Thermal designs of equipment where physical or chemical processes at boiling fluids are taking place desire the knowing of heat transfer coefficient. This field of study refers to the heat transfer coefficient determination, especially at technological important solutions and mixtures, volatile oils, etc. The boiling heat transfer in packed spaces will also be studied.

Since 1965, theoretical and practical investigations were made in order to realize high performance equipment which can be used in experimental determination. Simple equations for heat transfer coefficients calculation at boiling solutions and mixtures were established, as well as the process intensification through vibration, pulsation and stirring.

#### **RESEARCH TEAM**

Vasile Pode

#### **Researches in MAGNETIC FLUIDS: PREPARATION, CHARACTERISTICS AND UTILIZATION**

Magnetic fluids are obtained through magnetic precursor precipitation, followed by stabilization and magnetic particles dispersion. Studies for ultracentrifugation stability, rheological and surface phenomena characterization were made.

Theoretical and practical investigations were made for the preparation, characterization of the magnetic fluids. Ultracentrifugation stability and rheological characterization of the magnetic fluids were made. The results were concrete in design of magnetic

fluids processes and plants, as well as in magnetic fluids application and the nonmagnetic materials separation.

#### **RESEARCH TEAM**

Zeno Gropsian, Romulus Minea, Lazăr Gabor, Doina Gabor, Andra Tămaş

#### **Researches in COORDINATIVE COMPOUNDS ANALOGOUS TO THE REINECKE**

Studies regarding the exchange of ligands in the thiocianato-chrom (III) complexes as well, as studies of the spectra and kinetics of the solvolysis and thermal stability of the new synthesized compounds (analogous to the Reinecke) have been made.

The use of the new Reinecke analogous has been studied and solved as analytical reagents in the technological and qualitative control of the final products in the drug industry, in that of polyurethane foams and that of dye-stuff, with the aim of quantitative determination of metal ions, etc.

#### **RESEARCH TEAM**

Ilie Julean, Maria Pârlea, Mircea Ştefănescu, Rodica Unc, Cornelia Muntean, Marcela Stoia

#### **Researches in HOMO - AND HETEROPOLYNUCLEAR COMPOUNDS WITH ORGANIC LIGANDS**

Synthesis and characterization of some inorganic compounds used in analytical chemistry in order to obtain simple and mixed oxides with catalytic, pig mental and magnetic properties.

New analytical reagents have been prepared for halides and medical substances synthesis. 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**

Ilie Julean, Mircea Ştefănescu, Mihail Bîrzescu, Mircea Niculescu

#### **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 polymer-analogous reactions, synthesis of polymer-grafted tertiary heterocyclic amines acting as "hybrid-phase" 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, Maria Poraicu, Cornelia Păcurariu, Erika Reisz

#### **Researches in PHYSICAL CHEMISTRY. THE 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) hydroxide co precipitation; d) calcinations of mixture of salts and/or oxides. The reactivity of the systems was studied comparatively for the different synthesis methods used.

#### **RESEARCH TEAM**

Cornelia Păcurariu, Ioan Lazău

#### **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

#### **Researches in ELECTROCATALYSIS**

Obtaining, characterization and application of electrodes with catalytic activity.

Methods of the obtainment of electro catalytic films have been elaborated in the lab based on the thermal decomposition of some complex compounds and through thermal arc spraying technique. These films have been characterized through scanning electronic microscopy, X-ray diffraction and voltammeter. 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

#### **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 method, scanning electronic 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 Duţeanu

#### **Researches in SYNTHESIS OF CERAMIC RAW MATERIALS THROUGH HYDROSILICATE FORERUNNERS**

Using of the 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 Timișoara 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, Romul Marius Jurca, Radu Lazău

#### **Researches in STUDIES AND PROJECTS FOR THERMOTECNICAL INSTALLATIONS OF THE SILICATES INDUSTRY**

Studies upon the optimization of the thermal insulation of industrial kilns for the silicates industry and practical applications of the new solutions.

Conception of a program and database for intermittent and continuous kilns thermal insulation and their use in practical applications.

**RESEARCH TEAM**

Dumitru Becherescu, Nicolae Burtan

**Researches in REFRACTORY AND HEAT INSULATION MATERIALS FOR HIGH TEMPERATURE**

Conception and development of new high refractoriness bonding matrix for dense refractories; technologies for high temperature insulation materials (1500 -1800 °C).

Some results were presented in the communications: "Some aspects regarding the mechanism of bonding high – duty refractory grains with active mullite binder" and "Suspended roof – profitable solution in kilns construction".

A production technology for active mullite able to be used as bonding matrix for high refractory grains.

**RESEARCH TEAM**

Nicolae Burtan, Dumitru Becherescu

**Researches in FAST ION CONDUCTING GLASSES. REDOX EQUILIBRIA IN GLASSES. INVESTIGATIONS UPON NEW VITREOUS SYSTEMS**

Studies regarding fast ion conducting glasses and investigations upon new vitreous systems. Studies regarding redox equilibrium in binary vitreous systems for  $Mn^{2+}/Mn^{3+}$ ;  $Ti^{3+}/Ti^{4+}$ .

New fast ion conducting glasses were obtained. The influence of other transitional ions upon the global conductivity was studied. Glasses with optimal ion conductivity were design. 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 upon this equilibrium was studied. The influence of melting condition upon the presence of  $Ti^{4+}$  was studied, as well as its relationship with the iron present.

**RESEARCH TEAM**

Adina Lația, Cosmin Vancea

**Researches in MANUFACTURING OF SOME MULLITE – CORDIERITE AND HIGH ALUMINA TECHNICAL CERAMICS**

Studies on the realization of mullite – cordierite ceramics and high alumina ceramics by extrusion.

The influence of raw materials and sintering conditions, plastification of batches with organic forming aids and extrusion of thin walled profiles was investigated. Some results were presented in the communication: "Extrusion of thin wall profiles from mullite and mullite-cordierite type technical ceramics" at the Vth edition of "Academics Days of Timisoara". A second part of research – under

contract furnished a preliminary report to the beneficiary.

**RESEARCH TEAM**

Mihai Enache, Olga Gogu

**Researches in CHEMISTRY AND TECHNOLOGY OF CEMENTS WITH LOW FIRING TEMPERATURES**

The decrease of the firing temperature of the cements leads to a diminution of the energy consumption and to increase of the rotary kiln productivity.

The cements with low firing temperatures obtained had presented similarly characteristics to those of the standard Portland cement.

**RESEARCH TEAM**

Ioan Drăgoi, Aurel Ștefan Todinca

**RESEARCH PROJECTS**

1. CNCISIS Grant No 32940/2004, theme 26, code 531, type A: *Methanol – air fuel cells with skeleton nickel electrodes obtained by thermal arc spraying*

Value: 68,000,000 ROL

Director: Prof.dr.eng. Nicolae VASZILCSIN

Members: Prof. dr. eng. Corneliu DAVIDESCU  
Assoc. prof. dr. eng. Maria NEMEȘ  
Assist.eng.Andreea KELLENBEGER  
PhD student Mircea DAN  
PhD student Narcis DUȚEANU  
Master student Raluca DUMITRU  
Student Ovidiu FEIER  
Student Nadia POP  
Eng. Nicoleta PLEȘU  
Eng. Georgeta BLĂNUȚĂ

**FIELD DESCRIPTION**

The fuel cells seem to be a viable alternative source of energy for the future because of the high efficiency, acceptable cost and various applications. One of the major problems in fuel cells achievement which determines the efficiency and the consistence of these devices is the realization of the electrodes with the electro catalytic activity for the active reaction. The aim of the ground is the obtaining of new type skeleton nickel electrodes by thermal arc spraying technique suitable for methanol – air ( $O_2$ ) fuel cells.

**ACTIVITIES**

- Obtaining of electrodes by thermal arc spraying
- Activation of electrode by alkaline leaching of aluminum from nickel – aluminum layer
- Characterization of skeleton nickel by SEM, EDX and RX
- Specific area determination
- Methanol oxidation reaction study by voltammeter techniques

2. CNCSIS Grant No. 32940/2004, theme 3, code 536, type A: *Implementation of ecological production and ecodesign in drinking water treatment technologies*

*Value:* 57,000,000 ROL  
*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. Vasile 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  
 PhD student Marija LIKAREC  
 PhD student Mihaela ZAPARTAN  
 Student Ramona GHICA  
 Student Aniela POP  
 Student Corina HAIDUC

#### FIELD DESCRIPTION

Treatment technologies for drinking waters

#### ACTIVITIES AND RESULTS:

- The main objective consists of the reevaluation of processes from drinking water technology in order to obtain the ecological performances, by reaching of ecological production and ecodesign desiderate for obtaining especially of "safe drinking water" for human consumption
- Comparative studies and databases for national and international level regarding the disinfection methods for drinking water
- Strategies imposed in water drinking treatment in order to reach the ecological production
- Ecological transfer of these results to drinking eater plants of our country to align to both EU ecological standards and International Standardization Organization (ISO).

3. CNCSIS Grant No. 32940/2004, theme 15, code 535, type A: *Recovery and reuse technology of metallic ions from industrial waste for minimization pollution*

*Value:* 80,000,000 ROL  
*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  
 PhD student Alina CIRSTOIU  
 Student Alina POPA  
 Student Anamaria ANTON  
 Student Iosif CAREBA

#### 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 32940/ 2004, type A, theme , code: 208, *Strategies regarding the implementation of some depollution ecotechnologies of battered and critical soils*

*Value:* 37,000,000 ROL  
*Director:* Assoc. prof. dr. eng. Vasile PODE  
*Members:* Prof. dr. eng. Georgeta BURTICA  
 Prof. dr. eng. Eveline POPOVICI  
 Assoc. prof. dr. eng. Rodica PODE  
 Lecturer dr. eng. Adina NEGREA  
 Assist. eng. Florica MANEA  
 Assist. eng. Laura COCHECI  
 Eng. Corina MACARIE  
 Eng. Ovidiu FEIER

#### FIELD DESCRIPTION

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

- Monitoring, evaluation and control of highly polluted soils and of industrial wastes containing heavy metals;



- Identification of strategies for soil decontamination and their integration in economic cycle;
- Development of properly techniques for removal and neutralizing of dangerous compounds from polluted soils, taking into account new techniques by use of absorption and magnetic separation.

5. CNCSIS Grant No. 32940/2004, theme 1, code 38, type E: *Material base extention and research directions for laboratory from department research center*

*Value:* 200,000,000 ROL

*Director:* Prof. dr. eng. Georgeta BURTICA

*Members:* Prof. dr. eng. Aurel IOVI

Assoc. prof. dr. eng. Rodica PODE  
 Assoc. prof. dr. eng. Vasile 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  
 PhD student Marija LIKAREC  
 PhD student Mihaela ZAPARTAN  
 Student Ramona GHICA  
 Student Aniela POP  
 Student Corina HAIDUC

#### FIELD DESCRIPTION

The reference fields are environmental protection and engineering, with the research tasks: water treatment for drinking and industrial purposes; recovery treatment of wastewater and environmental analysis of industrial processes.

#### ACTIVITIES AND RESULTS:

- The Research Center Engineering of Water Protection and Depollution and Environmental Analysis of Industrial Processes, operated into "Politehnica" University of Timisoara frame.
- Our researches, for technologies improving and recovery of useful products and wastes, optimizing of water and wastewater treatment technologies, evaluation of environmental impact, control and pollution treatment, represents subjects of both master and PhD degree thesis, of scientific papers communicated at national and international conferences, published in national and international conferences, many basic and applied research projects.
- The requested equipments, in addition to those existing, will contribute to high degree development of research and teaching. Thus, similar conditions with those from developed countries will be attained.
- Instrumental conditions and their development, will assure properly research

and teaching conditions for Research Center members: professors, researchers, license, master and PhD students.

- We intend to realize laboratories of Research Center corresponding to requirements of SR EN ISO/CEI 17025 - 2001, underling the compatibilities with UE laboratories.

6. CNCSIS Grant 32940/2004, type TD: *Electrochemical sensors based on modified skeleton-nickel-polyaniline electrodes*

*Value:* 48,000,000 ROL

*Director:* Assist.dr.eng.Andrea KELLENBERGER

#### FIELD DESCRIPTION

The objective of this project was to obtain electrochemical sensors based on conductive polyaniline, with fast response time, improved stability and adherence between the electrodic substrate and the polymeric film. The application range of the electrochemical sensors based on modified skeleton-nickel-polyaniline electrodes envisage the potentiometric detection of anions, based on the ion exchange properties of polyaniline.

#### ACTIVITIES

- Preparation of the potentiometric sensor by electrochemical polymerization of aniline in acid media on the skeleton nickel substrate;
- Scanning electron microscopy, energy dispersive X-Ray and X-Ray diffraction characterization of the polyaniline film;
- Evaluation of the potentiometric response for the skeleton-nickel-polyaniline electrode towards different anions;
- Assessment of the selectivity coefficient for chloride anions in presence of iodide.

7. CNCSIS Grant 32940/ 2004, type Td: *Using the wastes from leather industry in the production of thermoresistant pigments with Cr (III) content*

*Value:* 65,000,000 ROL

*Director:* PhD student Radu-Ioan LAZĂU

#### FIELD DESCRIPTION

Starting from the actual facts in the country and abroad concerning the important amount of chromium containing wastes from leather industry, for which the actual disposing solutions are not satisfying anylonger and taking into account the pollution effect of the chromium compounds, the purpose of the present project is to turn to good these wastes in obtaining some oxide compounds with chromium content.

#### ACTIVITIES

- Establishing the Cr<sub>2</sub>O<sub>3</sub> content of the leather waste.
- Research study concerning the possibility of obtaining some spinel structure pigments

using the leather wastes as chromophore source.

- Synthesis of the designed thermo resistant pigments.
  - Characterization and testing of the obtained pigments.
8. AGRAL Program – PNCDI Project No. 169/2004: *Advanced Technology for Realization of premixuri with Chelate Microelements for Fast Application in Zootechny Field*

*Value:* 25,000,000 ROL

*Director:* Assoc. prof. dr. eng. Rodica PODE

*Members:* Prof. dr. eng. Georgeta BURTICA  
Assoc. prof. dr. eng. Vasile PODE  
PhD student Corina HAIDUC  
Student Ioana CORB  
Student Cristina COZEA

#### FIELD DESCRIPTION

The obtaining of new, high-performance mineral – vitamin premixture with macro and micro chelate elements for more species of animals, with zeolite volcanic tuff as basis support.

#### ACTIVITIES

- Elaboration and establishment of new technologies for obtaining of mineral premixuri with chelate macro and micro elements based on the interaction study between composition-synthesis conditions-structure- imposed biochemical properties
- Experimental working, technology and product obtaining in the laboratory
- Dissemination of the research results through participation at high-level national and international scientific meetings
- A presentation book will be edited
- Homologation, technology and product imposed

9. MATNANTECH Program – PNCDI Project no. 62/2001: *News geocomposites bentonitic materials used for hydro technical constructions and tightening of ecological wastes stores*

*Value:* 20,000,000 ROL

*Director:* Assist. eng. Laura COCHECI

*Members:* Assoc. prof. dr. eng. Petru NEGREA

*Value:* 20,000,000 ROL

*Director:* Assist.eng. Laura COCHECI

*Members:* Assist.eng. Eugen LUNGU  
CP I chem. Cornel BOGATU  
CP III eng. Ladislau ANDRES  
CP III eng. Valeria RUS  
CP III eng. Dan COCHECI  
Assist.eng. Florica MANEA  
Assoc.prof.dr.eng.PetruNEGREA  
CP III eng. Monica IHOS

Assist.eng. Marius GHEJU

Assoc.prof.dr.eng. Rodica PODE

#### FIELD DESCRIPTION

The development of a new technology and obtaining modern tightening materials, bentonitic geocomposites type, for hydro technical constructions and environmental protection.

The performances development of the Romanian tightening materials production.

#### ACTIVITIES

- Results of resistance determination due to chemical agents and degree of tightening for 3 types of bentonitic geocomposites, designed for tightening of ecological house wastes stores, are presented.
- EPA test 9090 was realized for 360 days using a levigate with presented composition, a simulation of tightening for more then 30 years of bentonitic geocomposites samples, both fixed and membrane type.

10. MENER Program – PNCDI Project no. 028/2001: *Reclamation possibilities and ecological approach of sterile within settling ponds under conservation*

*Value:* 60,000,000 ROL

*Director:* Assist. eng. Laura COCHECI

*Members:* Assist.eng. Eugen LUNGU  
CP I chem. Cornel BOGATU  
CP III eng. Ladislau ANDRES  
CP III eng. Valeria RUS  
CP III eng. Dan COCHECI  
Assist.eng. Florica MANEA  
Assoc.prof.dr.eng. Petru NEGREA  
CP III eng. Monica IHOS  
Assoc.prof.dr.eng. Rodica PODE

#### FIELD DESCRIPTION

Physical - chemical and mineralogical characterization of settling ponds under conservation. Proposals for stabilization and grass sowing as an ecological approach. The research concerning reclamation of raw sterile for building materials industry (prefabs).

#### ACTIVITIES

- The prefabs were tested for the evaluation of lixiviation characteristics.
- The laboratory experiments were carried out to establish whether heavy metals diffused from the hydraulic matrices.

### PhD RESEARCH ACTIVITIES

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

*PhD students:* Barbul Lucian, Barna Lucian, Bota Marcela, Dan Mircea, Duțeanu Narcis, Marian Eleonora, Holban Nina, Jurca Tunde, Niculescu Mircea, Popa Alexandru, Reisz Erika, Stoia

Marcela, Unc Rodica, Ursulescu Maria, Bota Marcela, Dippong Thomas, Ilici Maria

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

*PhD students:* Albulescu Gabriela, Bel Gabriela, Berbecea Adina, Bogatu Corneliu, Briea Carmen, Coheci Laura, Ghiga Mihaela Simona, Gheju Marius, Haiduc Corina, Ion Monica, Lungu Eugen, Magma Angela, Moravian Davila, Mice Daniela, Monrovia Claudia, Popes Elena, Romance Tamara, Rout Dan, Russ Adrian, Sebeka Moiré, Teuca Lavinia, Ursulescu Marius, Spartan Elvira Mihaela, Nagy Robert, Cîrstoiu Alina, Andon Mihaela, Lazău Carmen, Macramé Ioan, Russ Valeria, Maria Mihaela, Popa Florin

3. Prof. dr. eng. Delia PERJU, PhD supervisor in *Chemical Engineering*

*PhD students:* Calisevici Nicoleta, Cut Adina, Chicora Eugenie, Dumitrel Doru, Fiscal Monica, Levity Mirel, Manea Adele, Marinescu Sorin, Moldovan Raul, Pamfiloiu Mirabela, Pârlea Harieta, Osiceanu Antuaneta, Tănăsie Dan Cristian

4. Prof. dr. eng. Zeno GROPȘIAN, PhD supervisor in *Chemical Engineering*

*PhD students:* Borș Nicu, Brânzei Eugen, Ciubotariu Gheorghe, Coșoaba Bianca, Panescu Mihaela, Nadia Pop

5. Prof. dr. eng. Georgeta BURTIĂ , PhD supervisor in *Chemical Engineering*

*PhD students:* Podariu Camelia, Corb Ioana, Proca Cristina, Toader Mihaela, Macarie Amalia, Cical Elena, Jurj Luminița, Furdui Petru

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

*PhD students:* Bartiș Tihamer, Bejan Marius, Calapod Adriana, Călin Tațian, Lazău Radu, Neamțu Ion, Ziman Nicolae, Lupa Marius

7. Prof. dr. eng. Corneliu DAVIDESCU, PhD supervisor in *Chemical Engineering*

*PhD students:* Reisz Erika, Ardelean Radu, Peli Beata

8. Prof. dr. eng. Ioan LAZĂU, PhD supervisor in *Materials' Science and Engineering*

*PhD students:* Ecsedi Zoltan, Orban Alexandru

#### PHD THESIS SUSTAINED

1. Nina Holban: *Researches about the oxido – reduction reactions, photochemical catalyzed,*

*of the residual compounds with sulphur and hard metals from mining activities,* PhD supervisor Prof. dr. eng. Ilie Julean

2. Alexandru Popa, Base – *Catalyser interaction study in micro compounds oxide systems,* PhD supervisor Prof. dr. eng. Ilie Julean

3. Tunde Jurca, *Complex combinations of the pirazinamide and nicotinamide with transitional metals ions,* PhD supervisor Prof. dr. eng. Ilie Julean

4. Mircea Niculescu, *Complex combinations with addends oxidations products of the diols,* PhD supervisor Prof. dr. eng. Ilie Julean

5. Alexandrina Sim: *Synthesis of some oxidic compounds by unconventional methods,* PhD supervisor Prof. dr. eng. Dumitru Becherescu

6. Mihaela-Ioana Popovici: *Oxidic materials with directional properties,* PhD supervisor Prof. dr. eng. Dumitru Becherescu

7. Romul Marius Jurca: *Ceramic pigmys from hydro silicates precursors,* PhD supervisor Prof. dr. eng. Dumitru Becherescu

8. Andrea Kellenberger: *Study about the obtaining process of the skeleton electrodes by thermal pulverization method and their characterization,* PhD supervisors Prof. dr. eng. Aurel Iovi and Prof. dr. eng. Waltraut Brandl

9. Riviș Adrian, *Contributions to optimization and improvement of performances of hiperlipoproteinemia investigation methods,* PhD supervisor Prof. dr. eng. Delia Perju

10. Moșoarcă Giannin-Emanuel, *Contributions to the study for improvement of technological process for drinking water preparation by use of surface and ground waters,* PhD supervisor Prof. dr. eng. Delia Perju

11. Brusturean Gabriela-Alina, *Dépollution de sol par venting et extraction sous pression réduite: étude expérimentale, modélisation et simulation numérique,* PhD supervisor Prof. dr. eng. Delia Perju

12. Tămaș Andra Dana, *Contributions to Magnetic Fluids Preparation and Description – Emulsions with Magnetic Fluids Content,* PhD supervisor Prof. dr. eng. Zeno Gropșian

#### PUBLICATIONS

##### BOOKS

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6. Reisz, E., Sonntag, C., Davidescu, C.M., *Oxidation of Manganese(II) by Ozone in Strongly Acidic Media (pH = 0): Thermodynamic and Kinetic Aspects*, Chemical Bulletin of "Politehnica" University (Timișoara), 49 (63), 2004, pp. 55-60
7. Reisz, E., Sonntag, C., Davidescu, C.M., *Oxidation of Manganese(II) by Ozone in Neutral Aqueous Media in presence of polyphosphate: Thermodynamic and Kinetic Aspects*, Chemical Bulletin of "Politehnica" University (Timișoara), 49(63), 2004, pp. 61-66
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9. Sabou, R., Duțeanu, N., Bratu, D., Vaszilcsin, N., *The analysis of corrosion behavior in vitro of 8 ennobel dental alloys and the environment temperature influence on corrosion, (Romania language)*, Timisoara Medical Journal, vol. 54, supply. No. 2, ISSN 1583-5251, pp. 93 (abstract)

#### PUBLISHED PAPERS

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2. Lazău, I., Păcurariu, C., Kovacs, G., Lazău, R., Ionașcu, C., *Basalt Based Glass Ceramics. Kinetic Studies of the Crystallization Processes, Key Engineering Materials*, Trans. Tech. Publications, Switzerland, Vol. 264-268, pp. 1879-1882, 2004
3. Montana, C., Mărginean, G., Iovi, A., Negrea, P., *Study about thermal stability of ammonium-cobalt phosphates* (Romanian language), Chemistry Journal, 55(2), 2004, pp. 81-85
4. Vaszilcsin, N., Kellenberger, A., Magheț, T., Dumitru, R., Bîrzescu, M., Niculescu, M., *Crystalline structure of the product of thermal decomposition of polynuclear coordination compound  $[Ni(OH)_2(H_3CCH(OH)COO')_2(H_2O)_2 \cdot 0.5H_2O]_n$* , Chem. Bull. "Politehnica" Univ. (Timișoara), 49(63), 2004, pp. 72-75
5. Făgădar-Cosma, E., Făgădar-Cosma, Gh., Magda, A., *Displacement reactions of p-substituted acryldichloro-phosphines under the action of a nucleophile*, Chemical Bulletin of "Politehnica" University (Timișoara), 49 (63), 2004, pp. 25-28
10. Dan, M., Vaszilcsin, N., Kellenberger, A., Duțeanu, N., *Metal removal from dilute solutions using vibrating electrodes. II. Nickel removal*, Annals of the «Aurel Vlaicu» University of Arad, Series Chemistry, 2004, pp. 41-47
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14. Caizer, C., Ștefănescu, M., Barvinschi, P., *Unusual magnetic behavior of Nickel-Zinc ferrite nanoparticles in a silica matrix, obtained through the hybrid sol-gel method*, Annals of University of Petrosani, Physics, 6, 2004, pp. 111

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21. Caizer, C., Ştefănescu, M., Barvinschi, P., *Unusual magnetic behavior of nickel – zinc ferite nanoparticles in a silica matrix, obtained through the hybrid sol – gel method*, Annual Physics Conference, 13 – 14 Mai 2004, Petroşani, pp. 11 (abstract)
22. Dan, M., Vaszilcsin, N., Kellenberger, A., Duţeanu, N., *Metal removal from dilute solutions using vibrating electrode. III. Zinc removal*, Metal Elements in Environment, Medicine and Biology, 6-th International Symp. Timişoara, 8-10 Nov. 2004, pp.353-358
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33. Manea, F., Schoonman, J., Radovan, C., *Electrochemical Sensors for Environmental Monitoring*, First International Conference on Trends in Environmental Education EnvEdu, Brasov, 2004, pp.25
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38. Bogatu, C., Chiș, D., Botău, D., Ursoiu, I., Vlaicu, I., Iovi, A., Andres, L., *Some aspects concerning chlorine and chloramines analysis in water by use of DPD-FAS metod*, Proceedings of the 11<sup>th</sup> Symposium on Analytical and Environmental Problems, 27 Sept. 2004, Szeged, Hungary, ISBN 963-217-147-0, pp. 116
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43. Micu, D., Burtica, G., Likarec, M., Pode, R., *The Softening of the potable water utilizing chemical activated natural zeolites*, 35<sup>th</sup> International Scientific Symposium of Metra, 27-28 May 2004, Bucharest, ISBN: 973-03501-6, pp. 726-732
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47. Lazău, R. I., Becherescu, D., Păcurariu, C., Ianos, R., Kovacs, G., *Using wastes from Leather Industry as chromium source for ceramic pigments*, International Symposium on Inorganic and Environmental Materials, Eindhoven, Netherlands, 2004, pp.7
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- University (Timișoara), 49(63), 2004, pp. 149-151
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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 that 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
- Studies on structure-properties relationship using the topological model of organic molecules
- Structured packing 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

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### RESEARCH FIELDS

#### **New methods in organic synthesis**

*Keywords:* synthesis of organic compounds, carbonic acid derivatives, sterically hindered phenols with antioxidant activity, structure determination by NMR, biocatalysts 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 packing 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 auxiliaries



### 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, 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 phenolic antioxidants, studies of biocatalyst processes in organic synthesis and structure determination of organic compounds by NMR spectroscopy were also investigated.

#### RESEARCH TEAM

Carol Csunderlik, Maria Nutiu, 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 (haloderivatives, 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, Dan Hădărugă

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

The structured packing (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<sub>2</sub> 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 packing; 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 Stricatu, 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 Manovicu, Virginia Manovicu, Geza Bandur

### 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  $\chi$  and the Hildebrand

solubility parameter  $\delta$ ) 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 low-molecular 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 ( $\alpha,\omega$ -dihydroxy-polyesters). Chemical modification of polyethylene oligomers.

#### RESEARCH TEAM

Ionel Manovicu, Virginia Manovicu, Geza Bandur

#### 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 Boc, Ioan Macarie, Simona Popa

#### RESEARCH PROJECTS

1. CNC SIS Grant No 32940/2004, theme 14, code 20, type A: *Polyfunctional molecular models for polymer processing and tribological applications*

*Value:* 80,000,000 ROL

*Director:* Prof. dr. eng. Liviu MIRCI

*Members:* Dr. eng. Gheorghe ILIA

Dr. Phys. Paula LUCA

Eng. Lavinia MACARIE

Assist. eng. Sorina BORAN

Eng. Victor BOIANGIU

#### FIELD DESCRIPTION

Work deals with the synthesis and characterization of some polyfunctional derivatives built on the basis of citric acid. There were realized unsymmetrical as well as symmetrical triesters by taking into consideration aliphatic alcohols of variable length, up to 13 carbon atoms, along with special alcohols of a complex structure.

These special alcohols are derived from phenols with alkyl pendant groups of variable length and position through an ethoxylation reaction by using 1, 3 dioxolan-2-one (ethylene carbonate). The products obtained in this way present valuable properties either as polymer processing aids or as fluids with adequate properties to be used in the tribological field.

#### ACTIVITIES

The research done implied the following activities:

- synthesis, purification and characterization of the special alcohols of alkyl-aryl structure
- synthesis and characterization on the basis of specific organic indices of the unsymmetrical and symmetrical citric trimesters
- evaluation of the representative characteristics of the realized products as polymer plasticizers and as tribological fluids.

2. CNC SIS Grant No 32940/2004, theme 3-Ib, code 25, type AT: *Odorant and Flavoring Compounds – Molecular Modelling, Multivariate Analysis, QSAR*

*Value:* 66,000,000 ROL

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

*Members:* Assist. eng. Nicoleta HĂDĂRUGĂ

Student Ion BARBĂRASĂ

Student Bianca CRIȘAN

#### FIELD DESCRIPTION

Structure-Activity Relationships (SAR, QSAR, QSPR) in odorant-flavoring compound field are used only in the last years; the main problem is the primary mechanism of olfaction, many theories being proposed. It seems that the sterical and electronical parameters play a very important role in the ligand-receptor interaction. For this reason, finding the chemical space (physico-chemical

properties and structural descriptors) and the evaluation of the osmophoric map of the receptor sites in the odorant-flavoring compound field are very important goals. Developing the combinatorial synthesis and new methods for advanced search (VHTS-virtual high throughput screening) impose to build a flexible and compatible odorant-flavoring compound database. Using such databases statistically significant and useful QSARs can be obtained for different odor types and farther the "osmophoric" constellation of the receptor site could be evaluated and new odorant-flavoring compounds could be designed.

#### ACTIVITIES

An odorant database with 1486 compounds and a drug database containing 2000 compounds and 168 indices, characteristics and descriptors were built. A multivariate analysis (PCA-principal component analysis) on these databases provides a very good classification for these two types of organic compounds, especially for the physical properties.

The physico-chemical properties used in the databases building were collected from the literature, the structural descriptors were calculated using the 3D minimal energy conformation of molecules, and some GC and spectroscopic properties for 22 odorants, 37 essential oils and 83 flavoring systems were determined by GC-FID and GC-MS analysis. For 144 Maillard model systems the odorant composition was determined using the SH-GC-MS and MD-DH-GC-MS analyses a very good classification of the model systems being obtained by multivariate analysis.

From the odorant database two representative classes of odorant compounds were selected (sandalwood and musk odorants). A set containing 31 sandalwood odorants and structurally similar ones was used for obtaining QSAR models; the best results were obtained for specific hypermolecule *O*-group parameter and for the distance between the hydrophilic and hydrophobic centers of molecule as parameter ( $r = 0.88$ ).

In the case of musk odor, 86 compounds from the macrocyclic musk class and 47 compounds from the nitro- and non-nitro-aromatic musks were used in order to obtain SARs and QSARs, respectively. The best results were obtained in the case of MCD and  $\Delta E$  descriptors.

3. CNCSIS Grant 32940/2004, theme 6, code 135, type A: *Bis(O-Nitrophenyl) Carbonate, A Potential Reagent In Fine Organic Synthesis Included Combinatorial Chemistry And Asymmetric Synthesis (Carbonates, Polycarbonates, Carbamates, Oxazolidinones Synthesis*

*Value:* 80,000,000 ROL

*Director:* Prof. dr. chem. Carol CSUNDERLIK

*Members:* Prof. dr. eng. Mihai MEDELEANU  
Lect. dr. eng. Marius MILEA  
Assist. eng. Monika SIMON  
PhD student Andreea TARTA-MICLE  
PhD student Adina TÎRNEANU  
PhD student Adina SEGNEANU  
Student Ileana STETCO  
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.

#### ACTIVITIES

The research team performed the following investigation topics:

- The study of the reactions between bis (o-nitrophenyl) carbonate and various amines by FTIR spectroscopy in order to find the optimal conditions for obtaining the desired products.
- Synthesis and characterization of some new active o-nitrophenyl carbamates
- A study by X Ray diffraction of the nanostructure for some o-nitrophenyl carbamates
- Determination of the biologic activity of the carbamates obtained.
- Synthesis of some known ureeas using a new method which consists in using of bis(o-nitrophenyl) carbonate instead of phosgene.

4. CNCSIS Grant no. 32940/2004, theme 22, code 27, type A: *Continuous Frontal Polymerization*

*Value:* 130,000,000 ROL

*Director:* Assoc. prof. dr. eng. Lucian RUSNAC

*Members:* Lect. dr. eng. Geza Nicolae BANDUR  
Prof. dr. eng. Alfa Xenia LUPEA  
Lect. dr. eng. Carmen RUSNAC  
Lect. dr. eng. Francisc PETER

#### FIELD DESCRIPTION

The frontal polymerization is a technique of conversion of monomers into polymers in a restricted reaction zone (front) which propagate in the direction of the unreacted mixture of monomers. The rate of propagation of the front is determined by the initial temperature, the concentrations of monomers and initiators, and the viscosity of the reaction mixtures.

The main objective of the investigation is to develop a continuous reactor in which the front is stationary due to the pumping of monomers in the direction of the front with a rate equal to the rate of propagation of the front.

## ACTIVITIES

In the year 2003 the activities were centered on the following areas:

- Determination of the optimal conditions for the frontal polymerization: compositions of the mixtures of monomers and the influence of their nature on the rate of propagation of the front, initial temperature of the reactive mixture, influence of the diameter of the reaction tube on the rate of propagation, influence of the initiator concentration
- The postmixing effects of the structured packages and determination of the conditions which ensure piston flow in the postmixing zone
- The decomposing of initiators in columns equipped with structured packing in order to determine the composition of mixtures of initiator which give a constant concentration of radicals in the front

## PhD RESEARCH ACTIVITIES

1. Prof. dr. Carol Csunderlik, PhD supervisor

*PhD students:* Birò (Săcs -Birò) Emese, Kiss (Popa) Claudia, Tarța (Micle) Andreea-Romana, Laza Anca, Segneanu Adina, Tîrnăveanu Adina-Elena, Neanu Cristian, Fodor Catalin, Cseh Liliana, Belcea Monica, Stanoiev Zlatimir

2. Prof. dr. eng. Ionel Manovicu, PhD supervisor

*PhD students:* Stana Simona Maria, Florea Liliana, Șerban Claudia, Csak Gabriela, Boboicov Ecaterina, Pascu Cristian, Roșca Cristina, Homone Claudia, Sandu Maria, Gasparyl Ovidiu Virgiliu

3. Prof. dr. eng. Alfa-Xenia Lupea, PhD supervisor

*PhD students:* Voicu Marilena, Caciğ Svetlana, Cătănoiu Gabriela, Dumbravă Delia, Grad Maria, Lazăr Dorina, Vancea Valentina, Bebec Dana, Ionescu Carmen, Lascu Anca, Crâșmăreanu Elena, Szabo Rodica, Hădăruță Nicoleta, Samuilă Corina

4. Dr. eng. Dan Munteanu, PhD supervisor

*PhD students:* Boran Sorina

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