

## FOREWORD

The Faculty of Chemical and Food Technology of the Slovak University of Technology is one of the six faculties, of the Slovak University of Technology in Bratislava. The history of the Faculty dates back to 1940/41 when the Branch of Chemical Engineering started with education. The Higher Education Act from 1950 changed this branch to the individual Faculty of Chemistry of the Slovak Technical High School in Bratislava.

The Slovak higher education has its rich history. Our Faculty follows in the footsteps of its famous predecessor in the education of technical chemistry, i.e., the famous Mining Academy in Banská Štiavnica constituted by empress Maria Theresa in 1762. The establishment of the Dr. M. R. Štefánik College of Technology in 1937 and subsequently, that of the Slovak College of Technology in 1939 succeeded in keeping the high standard of technical education in Slovakia.

Within the time of its existence, the Faculty has educated more than 16 500 graduates (more than 3 600 graduates in food engineering). The Faculty has trained more than 1 100 graduates in postgraduate doctorate courses granting the title PhD in chemical and technical sciences. Thus, the Faculty has helped considerably to increase scientific knowledge in industry, education system, scientific and research institutes, and administrative services.

The Faculty occupies a very specific position within the Slovak Republic and relates to the whole spectrum of chemical, food, pharmaceutical and consumer industries, and ecology. At present, some 2.000 students study at the Faculty and they are trained by qualified pedagogical and research staff. Out of the total number of 273 teachers, there are 31 full professors, 106 associate professors, 139 assistant professors. Out of 85 research workers, 2 hold the title DSc, 45 hold the title PhD. Both the teaching process and research activities are centred within 24 Departments and Central Laboratories.

The Faculty currently offers study in BSc courses, MSc courses, and PhD. The undergraduate form of study is organized at two levels: Bachelor-of-Science and Master-of-Science programmes. The first level BSc course for all students lasts three years, and is run in two branches: Chemical Technology and Food Technology. This first level of the study ends by a state examination and a project granting the student the title Bachelor of Science (BSc). The nominal span of the study in the BSc course is 3 years. The second level MSc course is run in 9 majors with several possible specializations over two years. The MSc course ends by a state examination and by defending a diploma thesis. The graduate obtains the title Master of Science (MSc). In addition to the natural-science basis, students of all branches study basic engineering subjects, e.g. Chemical Engineering, Processes Control, Basics of Chemical and Food Processing Technology, as well as subjects on Economy, Law and Ecology.

The highest form of university education is currently the doctorate study, which in the past was run as a form of preparation for scientific work. In 1997 the Ministry of Education of the Slovak Republic approved the right of the Faculty to train and to administer examinations in PhD Courses. The Faculty has conferred the title PhD in 15 branches of the doctoral study. (Chemical Physics, Inorganic Chemistry, Organic Chemistry, Analytical Chemistry, Physical Chemistry, Macromolecular Chemistry, Biochemistry, Microbiology, Inorganic Technology and Materials, Organic Technology and Technology of Fuels, Technology of Macromolecular Materials, Chemical Engineering and Control of Processes, Chemistry and Technology of Environment, Chemistry and Food Technology, Biotechnology, and Applied Informatics).

The Faculty has a widely oriented programme, leading to the development of basic scientific fields in chemistry, chemical technology and food processing. This wide scientific orientation of Departments at the Faculty allows goal-oriented training of undergraduates and thereby their quicker transition to industry. There are several scientific schools at the Faculty which are successful at winning grants from domestic and international sources and at organising scientific meetings. The Faculty generally maintains an important international position. In addition to basic research, the Faculty participates in widely applied research for practice. The cooperation with many factories and companies allows for a swift application of research results in practice. At the same time the Faculty obtains considerable financial support.

The Faculty participates in issuing the specialized scientific journals: Chemical Papers, Fibres and Textile, Plastics and Rubber, Journal of Radioanalytical and Nuclear Chemistry, Biology, Folia Microbiologica, Vinohrad/Víno (Wineyard/Wine).

The scope and quality of the scientific activity keep the Faculty at a level, which is comparable with other top research and university centres in the world. This can be proved by the above mentioned number of grants, staff invitations to participate in conferences abroad, wide cooperation with foreign universities and institutions, and memberships in international organizations.

Any further details about the activities of the Faculty of Chemical Technology can be found in the Annual Report 2001.

February 2002

Prof. Vladimír Bálež, PhD, DSc  
Dean

## PRESIDIUM OF THE FACULTY

*Dean:* Prof. Vladimír Báleš, PhD, DSc

*Vice-deans:* Prof. Dušan Bakoš, PhD, DSc  
Assoc. Prof. Pavel Kovařík, PhD  
Prof. Ján Šajbidor, PhD, DSc  
Assoc. Prof. Zdenek Židek, PhD

## SCIENTIFIC COUNCIL

*Chairman:* Prof. Vladimír Báleš, PhD, DSc

*Vice-chairman:* Prof. Dušan Bakoš, PhD, DSc

*Members:* Prof. Stanislav Biskupič, PhD, DSc  
Prof. Dušan Bustin, PhD, DSc  
Assoc. Prof. Gabriel Čík, PhD  
Prof. Pavel Fellner, PhD, DSc  
Prof. Ľubor Fišera, PhD, DSc  
Prof. Milan Hronec, PhD, DSc  
Assoc. Prof. Pavel Kovařík, PhD  
Prof. Fedor Malík, PhD, DSc  
Prof. Milan Melník, PhD, DSc  
Prof. Ján Mikleš, PhD, DSc  
Assoc. Prof. Štefan Schmidt, PhD  
Assoc. Prof. Zdenek Židek, PhD  
Assoc. Prof. Tomáš Bleha, PhD, DSc  
Miroslav Havlík  
Assoc. Prof. Karel Kadlec, PhD  
Milan Kováč, PhD  
Ján Líška  
Prof. Anton Osvald, PhD  
Jozef Šimúth, PhD, DSc

*Honorary Members:* Milan Baláž  
Tibor Doboly  
Ondrej Gattnar, PhD  
Jozef Kollár  
Ján Maťaš  
Prof. Stanislav Miertuš, PhD, DSc

## ACADEMIC SENATE

*Chairman:* Assoc. Prof. Ján Dvoran, PhD.

*Vice-chairmen:* Assoc. Prof. Pavol Hudec, PhD  
Andrea Baránková, student

*Members:*

|                                     |                                   |
|-------------------------------------|-----------------------------------|
| Assoc. Prof. Ján Labuda, PhD, DSc   | Dr. Dušan Špirko, PhD             |
| Assoc. Prof. Marián Koman, PhD, DSc | Assoc. Prof. Viktor Milata, PhD   |
| Assoc. Prof. Jana Gabčová, PhD      | Štefan Šutý, PhD                  |
| Assoc. Prof. Soňa Jantová, PhD      | Zuzana Cvengrošová, PhD           |
| Assoc. Prof. Anton Gatíal, PhD      | Assoc. Prof. Mária Takáčsová, PhD |
| Assoc. Prof. Ivan Hudec, PhD        | Vladimír Kovár, PhD               |
| Vladimír Lukeš, PhD                 | Assoc. Prof. Anna Kolesárová, PhD |
| Milan Čertík, PhD                   | Viera Jančovičová, PhD            |
| Assoc. Prof. Jozef Markoš, PhD      | Ondrej Dolgoš, PhD-student        |
| Prof. Eberhard Borsig, PhD, DSc     | Rastislav Spišák, student         |
| Miroslav Hutňan, PhD                | Karol Caltík, student             |
| Assoc. Prof. Jozef Augustín, PhD    | Peter Ditte, student              |
| Tibor Jakubík, PhD                  | Pavol Lukáč, student              |
| Viliam Lendel, PhD                  | František Podzimek, student       |
| Assoc. Prof. Jozef Polonský, PhD    | Branislav Prosnan, student        |
| Pavel Kusý, PhD                     | Michal Tkáč, student              |

## DEPARTMENT OF ANALYTICAL CHEMISTRY

### Head of Department

Prof. Jozef Lehotay, PhD DSc

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### Full Professors :

Dušan Bustin PhD, DSc; Ján Krupčík, PhD, DSc, Jozef Lehotay, PhD, DSc, Eva Matisová, PhD, DSc, Ján Mocák, PhD, DSc

### Associate Professors :

Ernest Beinrohr, PhD, Eva Brandšteterová, PhD, Miroslav Čakrt, PhD, Ján Labuda, PhD, DSc, Drahomír Oktavec, PhD, Miroslav Rievaj, PhD, Jozef Polonský, PhD, Viktor Vrábel, PhD

### Assistant Professors :

Eva Benická, PhD, Tatiana Buzinkaiová, PhD, Andrea Hercegová, PhD, Elena Korgová, PhD, Pavol Májek, PhD, Alena Manová PhD, Pavol Tarapčík, PhD, Mária Vaničková, PhD

### Research Fellows :

Miriám Bučková, PhD, Adriana Ferancová, PhD, Katarína Hroboňová, PhD, Jarmila Laštincová, Jana Sádecká, PhD, Ivan Skačáni, PhD, Ivan Špánik, PhD, Peter Tomčík, PhD, Magdaléna Valachovičová

### PhD Students:

Branko Balla, Eva Blahová (till 1.10.2001), Jana Ďungelová, Peter Korytár, Petra Kotianová

### Technical staff :

Marta Benešová, Zuzana Cifrová, Jana Otrubová, Juraj Žemlička

## II. TEACHING AND RESEARCH LABORATORIES

Laboratory of capillary gas chromatography

Laboratory of high performance liquid chromatography

Laboratory of electroanalytical methods

Laboratory of molecular spectrometry

Clean laboratory for trace analysis with atomic spectrometry (AAS, OES-ICP)

Laboratory of organic elemental analysis

Laboratory of organic synthesis

Laboratory of fluorescence analysis

Laboratory of capillary isotachopheresis

Laboratory of electrochemical pre-concentration for atomic spectroscopy

Laboratory of chemometry

Laboratory of bioanalytical chemistry

## III. TEACHING

### A. Undergraduate Study

#### 4th sSemester

|                           |         |   |
|---------------------------|---------|---|
| Analytical Chemistry I.   | (2-2h)  | Beinrohr, Krupčík, Labuda, Polonský, Vrábel |
| Laboratory Practice AC I. | (0-4 h) | Valachovičová                               |

#### 5th semester

|                             |         |                                  |
|-----------------------------|---------|----------------------------------|
| Analytical Chemistry II.    | (2-2 h) | Bustin, Čakrt, Lehotay, Polonský |
| Laboratory Practice AC II.  | (0-4 h) | Korgová                          |
| Testing and Quality Control | (1-1 h) | Čakrt, Tarapčík                  |

#### 6th semester

Semestral Project

#### 7th semester

|  |         |                         |
|--|---------|-------------------------|
| Atomic Spectrometry                                | (2-0 h) | Beinrohr, Manová        |
| Anal.Chem.of Complex Inorg. Mixtures               | (2-0 h) | Oktavec, Polonský       |
| Anal.Chem. of Complex Org. and Biological Mixtures | (2-0 h) | Brandšteterová, Skačáni |
| Lab.Practice I.                                    | (0-1 h) | Matisová                |
| Biosensors   | (2-1 h) | Labuda, Mocák           |
| Computer evaluation of anal. measurement           | (2-0 h) | Májek, Mocák            |

#### 8th semester

|   |         |                    |
|---|---------|--------------------|
| Electrochemistry and Electro-analytical Chemistry | (2-1 h) | Bustin, Mocák      |
| Techniques of Mixtures Separation                 | (2-2 h) | Matisová, Valigura |
| Analytical Separation of Compounds                | (2-1 h) | Krupčík, Matisová  |
| Lab.Practice II                                   | (0-6 h) | Matisová           |

|  |          |                      |
|--|----------|----------------------|
| Nuclear Analytical Chemistry             | (2-0 h)  | Tarapčík, Májek      |
| Trace Analysis and Microanalysis Methods | (2-0 h)  | Beinrohr, Čakrt      |
| Environmental Analytical Chemistry       | (2-0 h)  | Benická, Buzinkaiová |
| Automatisation of Analytical Chemistry   | (2-0 h)  | Rievaj, Dzurov       |
| <b>9th semester</b>                      |          |                      |
| Bioanalytical Chemistry                  | (2-1 h)  | Labuda, Mocák        |
| Identification of Chemical Substances    | (2-1 h)  | Lehotay, Liptaj      |
| Lab.Practice V.                          | (0-1 h)  | Matisová             |
| <b>10th semester</b>                     |          |                      |
| Laboratory of Diploma Work               | (0-30 h) |                      |
| Selected Subjects                        |          |                      |

#### IV. CURRENT RESEARCH PROJECTS

##### A. Development and Application of Direct Injection Assays for HPLC Analysis of Some Drugs and Toxic Compounds in Biological Samples (Eva Brandšteterová)

The aim of the project was the development and the application of new assays with the possibility of direct injection of biological samples into the HPLC system. SPE (Solid Phase Extraction) precolumn was integrated directly into the HPLC system what improves validation parameter values and minimizes the personal contact with biofluids. Automated HPLC procedures for the analysis of chosen drugs, natural and toxic compounds were compared with applied electromigration methods.

##### B. New Electroanalytical and Spectroscopic Systems for Ultra-trace and Speciation Analysis with Special Emphasis to Environmental and Clinical Problems. Optimization of Analytical Procedures (Dušan Bustin)

The project was oriented to the development of analytical methods for ultratrace analysis of some biologically and environmentally important analytes. Flow - through galvanostatic chronopotentiometry has proved to become a calibrationless method for the determination of electrochemically active species. The method enables the measurement of extremely low (below  $\mu\text{g/l}$ ) as well as medium and high analyte concentrations, e.g. over  $\text{g/l}$ . The method provides reliable results and owing to its robustness it can also be applied for unattended monitoring of toxic species in waters. Porous electrodes facilitates the electrochemical generation of hydrides for their consecutive determination by atomic spectroscopy. Flow-through coulometry was successfully applied for the measurement of metal layer thickness. Using new chemometrical and statistical procedures, the original multidimensional analytical data were transformed into ulticomponents, which enable a detailed characterization of clinical, environmental or food samples. Thus, it was possible to find the way how the original chemical and physical parameters affect the main diagnostic features or desired properties of the analyzed subject or object. New chemometrical procedures were utilized for obtaining the resolution of the overlapped voltammetric signals as well as the modelling of the signal shape and height under different conditions of an electrochemical experiment. The IUPAC- recommended method for determining the limits of detection and quantification was reformulated in a new, more comprehensive way. This way applies easy calculation, however, it is still statistically perfect.

##### C. Development of selective methods for analysis of biologically active compounds by selected chromatographic and electroanalytical methods (Ján Krupčík)

This project intends to contribute to development of methods for: (a) Computer assisted optimization of chromatographic separation of mixtures of biologically active compounds in several columns coupled in series under multicolumn and multidimensional separation conditions, (b) Modeling of gas-chromatographic separation and explanation of chiral recognition of enantiomers in gas chromatography on chiral columns using knowledge and data obtained by theoretical chemistry (semiempirical and "ab initio" methods) and by structure -retention data correlations for enantiomers of analyzed compounds. (c) Computer assisted signal processing for deconvolution together with an increase of signal to noise ratio of weak signals which are not resolved experimentally. Elaborated algorithms shall be exploited for processing of signals in gas chromatography and electroanalytical methods. Procedures for the determination of uncertainties and evaluation of signal errors shall be implemented in elaborated algorithms, too. (d) Analytical characterization and application of new types of chemical modifiers for electrodes, based on DNA, proteins and substances with the chiral properties.

##### D. Trace analysis of selected analytes in complex organic systems by combination of preconcentration techniques and capillary gas chromatography. (Eva Matisová)

The project is oriented to the development of methods for the trace analysis of selected, particularly volatile and semivolatile compounds in complex organic systems - in environmental matrix utilising preconcentration techniques in combination with capillary GC. A part of the project is devoted to the miniaturisation in analytical chemistry

- to the development of microextraction methods for the sample preparation, large volume injection in capillary GC. A part of the project is connected with the development of high speed GC
- devoted to trace analysis.

##### E. The development of modern method for teaching analytical chemistry supported by PC (Pavel Tarapčík)

The main drawbacks of traditional teaching method of analytical chemistry are: low individual activity of students in classroom; unified work rhythm not considering individual abilities of students; low variability; high cost of modern laboratory method. There is a possibility to overcome these drawbacks applying relatively individual work in front of PC. The main goals of this project are:

- to provide simulating software for various analytical methods, mainly in the area of chemical equilibria in analytical chemistry,
- to provide teaching procedures supported by simulating software, combining work methods in whole group by traditional method and in small groups (two-three students) with PC.

The spreadsheet „EXCEL“ is widely used calculating product with high poverty of graphics, statistics..., the supporting software will be made on this basis as the EXCEL sheets, partly with macros in VBA language.

## V. COOPERATION

### A. Cooperation in Slovakia

Department of Microelectronics Faculty of Electrical Engineering and Information Technology, Slovak University of Technology Bratislava

Department of Petroleum Technology, Department of Biotechnology and Environment, VURUP, Slovnaft a.s. Bratislava

Department of Plant Physiology, Faculty of Natural Sciences, Comenius University, Bratislava

Faculty Hospital, Bratislava

Food Research Institute, Bratislava

Hospital for Tuberculosis and Respiratory Diseases, Department of Clinical Chemistry, Kvetnica, 058 87 Poprad

Hospital of the Ministry of Defence, Division of Clinical Laboratories, 833 31 Bratislava

National Institute of Oncology, Bratislava

Pharmaceutical Faculty, Comenius University, Bratislava

Slovak Institute of Metrology, Karloveská 63, 842 55 Bratislava

### B. International Cooperation

Department of Analytical Chemistry, Chemical Technological Faculty, University, Pardubice, Czech Republic

Department of Analytical Chemistry, Palacky University, Olomouc, Czech Republic

Department of Environmental Chemistry and Ekoanalytics, Faculty of Chemistry

Department of Chemistry, Gilman Hall, Iowa State University, Ames, Iowa, USA

Chiral separation of optical active compounds by HPLC and HRGC

Department of Organic Chemistry, University of Gent, Gent, Belgium

Chiral separations by HRGC

Faculty of Material Engineering and Ceramics, The University of Mining and Metallurgy, Al. Mickiewicza 30, 30-059 Cracow, Poland

Institut de Physique Nucléaire, 91406 Orsay Cedex, France

Institute of Pharmaceutical Chemistry, University of Muenster, Germany

Nicholas Copernicus University, Toruń, Poland

Prof. Hans Puxbaum; Technical University Vienna, Institute of Analytical Chemistry, Vienna, Austria

Utilisation of Capillary GC in Combination with Preconcentration Techniques for the Analysis of Organic Compounds in Aerosols

### C. Membership in Domestic Organizations and Societies

Chairman of Scientific Group "Chromatography and Electrophoresis",

Slovak Chemical Society, Slovak Academy of Sciences, Bratislava

(E. Brandšteterová)

Chemical Papers Editorial Board

(D. Bustin)

Membership in the Editorial Board of the Slovak scientific journal

Laboratory Diagnosis

(J. Mocák).

Slovak Chemical Society at Academy of Science, Group of

Analytical Chemistry

(J. Krupčík)

Slovak Chemical Society at Academy of Science, Group of

Analytical Chemistry

(J. Lehotay)

Slovak Chemical Society

(D. Bustin)

Slovak Society of Clinical Biochemistry. ISSN 1335-2644

(J. Mocák)

### D. Membership in International Organisations and Societies

American Chemical Society

(D. Bustin)

European Commission, Science, Research and Developments

(J. Lehotay)

Chemical Analysis Editorial Board

(J. Lehotay)

IUPAC

(D. Bustin)

UICC (International Union Against Cancer), Geneva, Switzerland

(Eva Brandšteterová)

### F. International Scientific Programmes :

Grant No. 002-98, Slovak – US Universities Co-operation. Mechanistic study of chiral recognition in HPLC and HRGC (J. Krupčík). The main objective of the project is to study mechanistic aspects of chiral recognition in the direct separation of enantiomers by HPLC and HRGC. The influence of structure and polarity differences in substituents bonded to the asymmetric carbon atom in enantiomers, and selectivity of a chiral selector in HPLC and HRGC shall be studied in detail. Elaborated optimum separation system shall be used for two dimensional separation of optically active compounds in natural samples.

### G. Visitors from Abroad

Prof. D.W.Armstrong

Department of Chemistry, Gilman Hall, Iowa State University, Ames, Iowa, USA, August 2001 (5 days)

Prof. Andrzej Bobrowski, DSc.

The University of Mining and Metallurgy, Cracow, Poland, March 2001 (10 days)

Prof.A.Manschreck

Department of Organic Chemistry, University of Regensburg, Germany

Prof.P.Sandra

Department of Organic Chemistry, University of Gent, Gent, Belgium, August 2001 (5 days)

Dr. Matija Strlič

The University of Ljubljana, Ljubljana, Slovenia, January-February 2001 (44 days)

**H. Visits of Staff Members and Postgraduate Students in Foreign Institutions**

|              |   |
|--------------|---|
| B. Balla     | Prag, Czech Republic, May 31 2001 (1 day)                     |
| B. Balla     | Austria, June 10-30 2001 (21 days)                            |
| E. Beinrohr  | Gent, Belgium, February 10-13 2001 (4 days)                   |
| E. Beinrohr  | Budapest, Hungary, February 27 2001 (1 day)                   |
| E. Beinrohr  | Fridek – Mistek, Czech Republic, June 12 2001 (1day)          |
| E. Beinrohr  | Czech Republic, conference, November 13-14 2001 (2 days)      |
| M. Bučková   | Dortmund, Germany, February 15 – May 14 2001 (1 month)        |
| M. Bučková   | Dortmund, Germany, September 3 – November 2 2001 (2 months)   |
| M. Čákr      | Fridek-Mistek, Czech republic, June 12 2001 (1day)            |
| J. Ďungelová | Czech Republic, November 19 – December 19 2001 (1 month)      |
| A. Ferancová | Czech Republic, January 5 – January 31 2001 (1 month)         |
| A. Ferancová | Czech Republic, conference, June 19–23 2001 (5 days)          |
| A. Ferancová | Prag, Czech Republic, July23 – August 18 2001 (1month)        |
| S. Hrouzková | Sophia, Bulgary, June 6-10 2001 (5 days)                      |
| P. Korytár   | Deutschland, January 1 December 31 2001 (12 months)           |
| P. Kotianová | Wien, Austria, January 29 2001 (1 day)                        |
| P. Kotianová | Wien, Austria, January 31 2001 (1 day)                        |
| P. Kotianová | Wien, Austria, March 1 2001 (1 day)                           |
| P. Kotianová | Las Vegas, USA, conference, May 18-28 2001 (11 days)          |
| P. Kotianová | Wien, Austria, May 4 2001 (1 day)                             |
| P. Kotianová | Wien, Austria, June 29 2001 (1 day)                           |
| P. Kotianová | Wien, Austria, July 31 2001 (1 day)                           |
| J. Krupčík   | Wien, Austria, conference, January 23-24 2001 (2 days)        |
| J. Krupčík   | Belgium, conference, May 27 – June 2 2001 (7 days)            |
| J. Krupčík   | USA, conference, July 10–23 2001 (14 days)                    |
| J. Krupčík   | Bruxelles, Belgium, conference, September 17–22 2001 (7 days) |
| J. Krupčík   | Deutschland, conference, October 7–10 2001 (4 days)           |
| J. Krupčík   | Bruxelles, Belgium, November 14–16 2001 (3 days)              |
| J. Krupčík   | Paris, France, conference, December 3–6 2001 (4 days)         |
| J. Labuda    | Czech Republic, June 19–23 2001 (5 days)                      |
| J. Labuda    | Deutschland, September 29 – October 5 2001 (8 days)           |
| J. Labuda    | Czech Republic, November 1–2 2001 (2 days)                    |
| J. Labuda    | Czech Republic, November 14–16 2001 (3 days)                  |
| J. Labuda    | Czech Republic, November 27–December 1 2001 (5 days)          |
| J. Lehotay   | Wien, Austria, conference, January 23-24 2001 (2 days)        |
| J. Lehotay   | Czech Republic, conference, May 22–25 2001 (4 days)           |
| J. Lehotay   | Danmark, conference, June 4–7 2001 (4 days)                   |
| J. Lehotay   | Czech Republic, conference, June 12–14 2001 (3 days)          |
| J. Lehotay   | USA, conference, July 10–23 2001 (14 days)                    |
| J. Lehotay   | Siofok, Hungary, September 1–5 2001 (5 days)                  |
| J. Lehotay   | Poland, September 19–21 2001 (3 days)                         |
| J. Lehotay   | Deutschland, conference, October 7–10 2001 (4 days)           |
| J. Lehotay   | Czech Republic, October 30 2001 (1 day)                       |
| J. Lehotay   | Belgium, November 14–16 2001 (3 days)                         |
| E. Matisová  | Spain, conference, May 9-18 2001 (10 days)                    |
| E. Matisová  | Wien, Austria, June 29 2001 (1 day)                           |
| E. Matisová  | Deutschland, conference, October 7-10 2001 (4 days)           |
| J. Mocák     | Brno, Czech Republic, May 23-24 2001 (2 days)                 |
| J. Mocák     | Graz, Austria, June 15–30 2001 (15 days)                      |
| J. Mocák     | Poland, September 14–21 2001 (8 days)                         |
| P. Oswald    | Gent, Belgium, February 6 - July 5 2001 (5 months)            |
| I. Špánik    | USA, August 1 – December 31 2001 (5 months)                   |
| A. Žiaková   | Pardubice, Czech Republic, June 18-19 2001 (2days)            |

**VI. THESES AND DISSERTATIONS****A. Graduate Theses (MS Degree) for state examinations after five years of study in Analytical Chemistry (Supervisors are written in brackets)**

|                 |   |
|-----------------|---|
| Adamcová Z.:    | HPLC ultratrace analysis of some nitroaromatics compounds in soil samples (K. Hroboňová)  |
| Baranová V.:    | Analysis using DNA biosensor (J. Labuda)  |
| Blahová. E.:    | The study of sorbents of new generation in sample-handling before HPLC analysis of morphine and its metabolites (E. Brandšteterová) |
| Čonka K.:       | Extraction of persistent organic compounds from biological samples using the methods of SPE (A.Kočan)                               |
| Gašpířiková K.: | Study of the sorption of some cations on the teflon surface (P. Tarapčík)   |
| Heldiová E.:    | In – electrode coulometric titrations: determination of some metals (E. Beinrohr)   |

|                    |  |
|--------------------|--|
| Hrašková L.:       | Preparation and application of DNA modified electrode. (M. Vaničková)  |
| Krascsenits Z.:    | Determination of fluorides in waters (M. Čákrť)  |
| Krištof J.:        | Detailed twodimensional and multidimensional data analysis (J.Mocák)   |
| Malychová Z.:      | Isotachophoretic determination of citric and isocitric acid (J. Sádecká)   |
| Martinkovičová K.: | In – electrode coulometric titrations: determination of acids and bases (E.Beinrohr)   |
| Rexová D.:         | Application of microelectrodes in voltammetric analysis (M. Rievaj)  |
| Senková Z.:        | Rojkovičová T.: The HPLC separation of some enantiomers using macromolecules of antibiotics as stationary phase (J. Lehotay) |
| Skaličanová A.:    | Determination of antidepressive drugs and pollutants using electrochemical biosensors (E. Korgová)                           |
| Slaná I.:          | Electroanalytical application of interdigitated microelectrodes arrays (D. Bustin)   |
| Šimeková M.:       | Determination of phosphates in waters by flow –trough coulometry (A. Manová)   |
| Škrabáková Z.:     | Fast gas chromatography and its utilisation in the analysis of organic compounds (E. Matisová)                               |
| Štorcel M.:        | Optimization of the Determination of High Boiling Petroleum Hydrocarbons by UV and IR Spectrometry (D. Oktavec)              |
| Tóthová A.:        | Possibility of determination some chosen drugs by capillary isotachopheresis (T. Buzinkaiová)                                |
| Verčík T.:         | Crystal structure and biological activity of 1,4 dihydropyridine derivatives (V.Vrábel)                                      |
| Žabka M.:          | The analysis of persistent organic contaminants in food products (E. Benická)  |
|                    | Optimization of separation of enantiomers by dual column capillary gas chromatography in chiral columns (J. Krupčík)         |

## B. Dissertations (PhD)

|               |  |
|---------------|--|
| Ferancová A.: | Development and utilization of sensors based on $\beta$ - cyclodextrin modified electrodes (J. Labuda)   |
| Hercegová A.: | Utilization of some electromigrating methods in pharmacy ITP determination of some selected nonsteroidal antirheumatics in body fluids and pharmaceutical preparations (J. Polonský) |

## VII. PUBLICATIONS

### A. Journals (\* registered in Current Contents)

- [1]\* Balla B., Mocák J., Pivovarníková H., Balla, J., Kavková D., Varmusová E.: Application of Multivariate Analysis in Laboratory Medicine. Clin. Chem. Lab. Sci. 39, 285 (2001)
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**C. Books and Textbooks**

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**D. Patents****E. PC Programmes**

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- [2] Tarapčík P.: Programs supporting teaching of instrumental analysis AC2 (2001)
- [3] Tarapčík P.: Kalib - General procedure of the result solution via linear calibration method with uncertainty evaluation (2001)
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- [5] Tarapčík P.: Simul-ch dynamic simulation and presentation of separation process in chromatographic column, useful for explanation of the influence of various parameters of separated mixture and experimental conditions on final chromatographic output (2001)
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## DEPARTMENT OF BIOCHEMICAL TECHNOLOGY

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**Associate Professors:**

Michal Rosenberg, PhD, Daniela Šmogrovičová, PhD, Ernest Šturdík, PhD

**Assistant Professors:**

Katarína Dercová, PhD, Zoltán Dömény, PhD, Helena Hronská, PhD, Mária Šturdíková, PhD

**Research Fellows:**

Milan Čertík PhD, Ľudmila Krištofiková, Dušan Slugeň, PhD, Valter Vollek, Marián Navrátil, PhD

**PhD students:**

Katarína Furdíková, Lucia Sláviková, Milan Valach, Igor Voštiar, Roman Tandlich

**Technical Staff:**

Vlasta Sládková, Jaroslava Telgárska

### II. TEACHING AND RESEARCH LABORATORIES

#### A. Teaching Laboratories:

Laboratory for the design of bioactive compounds  
Laboratory for biotechnological production of organic acids and fine chemicals  
Laboratory for study, isolation and transformation of microbial lipids  
Laboratory of secondary metabolites  
Laboratory of wine microbiology and oenology  
Laboratory of bioengineering  
Laboratory for solid-state fermentations  
Laboratory of yeast biotechnology  
Laboratory for microbial degradation of xenobiotics  
Laboratory of brewery technology

### III. TEACHING

#### A. Undergraduate Study

**3rd semester (autumn)**

|                               |           |         |
|-------------------------------|-----------|---------|
| Biochemistry and Microbiology | (2-1-0 h) | Šturdík |
|-------------------------------|-----------|---------|

**5th semester (autumn)**

|                             |           |         |
|-----------------------------|-----------|---------|
| Principles in Biotechnology | (2-0-0 h) | Malík   |
| Xenobiochemistry            | (2-0-0 h) | Dercová |

**6th semester (spring)**

|                       |           |   |
|-----------------------|-----------|---|
| Biophysical Chemistry | (2-2-0 h) | Valko, Voštiar  |
| Semestral Work        | (0-0-4 h) | Dömény, Čertík, Hronská, Navrátil,<br>Šmogrovičová, Šturdík, Šturdíková |

**7th semester (autumn)**

|  |             |  |
|--|-------------|--|
| Enzymology and Enzyme Engineering              | (2-2-0 h)   | Augustín, Hronská  |
| Biochemical and Biotechnological Informations  | (1-2-0 h)   | Šmogrovičová, Dömény, Navrátil   |
| Technical Microbiology                         | (2-0-0 h)   | Šturdík  |
| Biosynthesis and Transformation of Metabolites | (2-0-0 h)   | Rosenberg  |
| Special Laboratory                             | (0-0-3-4 h) | Čertík, Dömény, Hronská, Rosenberg,<br>Šmogrovičová, Šturdík, Šturdíková |

**8th semester (spring)**

|                                     |           |  |
|-------------------------------------|-----------|--|
| Bioanalytical Methods               | (2-1-0 h) | Šajbidor                                   |
| Laboratory of Bioanalytical Methods | (0-0-2 h) | Hronská, Sláviková, Navrátil, Tkáč, Zigová |
| Bioengineering                      | (2-2-0 h) | Polakovič, Slugeň                          |
| Pharmaceutical Biotechnologies      | (2-0-1 h) | Šturdíková                                 |

|   |                        |  |
|---|------------------------|--|
| Ecochemical Biotechnologies<br>Special Laboratory | (2-0-1 h)<br>(0-0-6 h) | Rosenberg, Dercová<br>Čertík, Dercová, Dömény, Hronská, Navrátil,<br>Rosenberg, Šmogrovičová, Šturdík, Šturdíková  |
| <b>9th semester (autumn)</b>                      |                        |  |
| Food Biotechnology                                | (2-0-1 h)              | Malík, Slugeň  |
| Malting and Brewing                               | (2-0-1 h)              | Šmogrovičová, Dömény   |
| Chemistry and Microbiology of Wine                | (2-0-1 h)              | Malík, Volleková   |
| Microbial Biomass and Distillery                  | (2-0-1 h)              | Šmogrovičová, Augustín   |
| Biochemical and Genetical Regulations             | (2-0-1 h)              | Šturdík, Dömény  |
| Special Laboratory                                | (0-0-6 h)              | Čertík, Dercová, Dömény, Krištofiková, Malík,<br>Navrátil, Rosenberg, Slugeň, Šmogrovičová,<br>Šturdík, Šturdíková |
| <b>10th semester (spring)</b>                     |                        |  |
| Diploma Work                                      |                        |  |
| <b>B. PhD Study</b>                               |                        |  |
| Biochemical Technology                            | (3 h)                  | Augustín   |

#### IV. CURRENT RESEARCH PROJECTS

##### A. Application of microorganisms in food industry and agriculture – biotechnological aspects. (Ján Šajbidor)

Yeasts (*Saccharomyces cerevisiae*) important for the production of Tokay type wines were isolated. We have isolated ethanol and osmo- tolerant strain *Saccharomyces cerevisiae* suitable for very high gravity wort fermentation, too. The strain was immobilised on a new type of hydrogele and it was successfully tested in large-scale pilot experiments. Patented process of non-alcoholic beer production based on wort fermentation by mutant strains with defective enzymes in Krebs cycle can be assumed as an original result of our research. Contaminated soil near former operation for polychlorinated biphenyl production - Chemko Strážske - was a source for isolation of *Alcaligenes xylosoxid* and *Pseudomonas stutzeri* bacteria strains useful for bioremediation technologies. Valuable results were presented in papers deals with relationship between structure of xenobiotics and their biodegradability. A new isolate identified as *Nocardia* species with high activity of cis-epoxysuccinat dehydrogenase was developed for food industry. This patented strain is deposit in the Czech Collecion of Microorganisms (CCM). We suppose its application in tartaric acid production by fermentation process. This problem was solved in cooperationin with BCS Engineering Ltd. Activity of fumarase in our producer *Dipodascus magnusii* - enzyme for malic acid production by fermentation of sugar medium - have been approximately ten times higher in comparison with earlier published data. We suppose application of this solution in industrial production of malic acid similiary as former mentioned result. Monitoring of biotechnology processe via application of biosensors was in the focus of our interest, too. New types of biosensors based on electrochemistry or microcalorimetry principles for monitoring of ethanol production from sucrose, glucose, lactose or biotransformation of glycerol to dihydroxyacetone was published in scientific journals. Individual part of our research is overproduction of secondary metabolites for food industry and pharmacy. We have isolated new metabolite of *Penicillium funiculosum* called OR-1 having inhibition effect against proteinase trypsin. This fact can be used in pharmacy and medicine. New trends in fortification of cereals with essential fatty acids via solid-state fermentations (for human nutrition or animal feed) were published. Very interesting result were obtained during the study of lipogenesis regulation in filamentous fungi.

##### B. Immobilized technologies: Implementation of new immobilization techniques/technologies into microbial and plant fermentations and biotransformations and their industrial applications (Ernest Šturdík)

The project aims to integrate up-to-date knowledge of material engineering of supports (new hydrogels and composite materials for capsule cell immobilization, new methods of exact measuring of mechanical properties of hydrogel supports), immobilization methods (new gelation techniques), methods of preparation of immobilized cells with uniform size and shape in volumes needed for industrial application, knowledge of effect of immobilization process to physiological state and metabolism of cells and microbial and plant fermentation biotechnologies, biotransformations and xenobiotics biodegradations. The most perspective are: fermentation of starch hydrolysates to ethanol, primary and secondary beer fermentation, tensid-like xenobiotics degradation.

One of the main aims of the project has been to test the selected variety of hydrogels and other composite materials for cell immobilization by techniques of entrapment and encapsulation. These should be applied in fermentation technologies applicable in industrial praxis. Yeast cells were used when immobilized in hydrogels (alginate, pectate, carrageenan) and other synthetic polymers (polyvinyl alcohol) and tested in fermentation processes under batch, semi-continuous and continuous conditions. Electrochemical and microcalorimetric biosensors have been constructed and successfully applied to monitor the processes.

#### V. COOPERATION

##### A. Cooperation in Slovakia:

VÚL Modra  
Institute of Drug Research, Modra  
Soil Science and Conservation Research Institute, Bratislava  
Institute of Preventive and Clinical Medicine, Bratislava  
Faculty of Pharmacy, Comenius University, Bratislava  
Institute of Experimental Pharmacology, Slovak Academy of Science, Bratislava  
Institute of Ecobiology, Slovak Academy of Science, Bratislava

Institute of Chemistry, Slovak Academy of Science, Bratislava  
 Institute of Experimental Endocrinology, Slovak Academy of Science, Bratislava  
 University Cyril and Methods, Trnava  
 Likospol, Bratislava  
 Allcop, Bratislava  
 Research Institute of Viticulture and Oenology, Bratislava  
 Brewery, S.t.e.i.n., a.s., Bratislava  
 Brewery, Codecon, Svätý Jur  
 Wine Establishments in Bratislava-Rača, Pezínok, Sered', Nitra, Tibava  
 Slovakofarma, Hlohovec  
 Biotika, Slovenská Ľupča  
 Topvar Brewery, Topoľčany  
 Codecon, Sv.Jur  
 Biopo, Leopoldov  
 Research Institute of Rheumatic Diseases, Piešťany  
 Piešťany spa  
 Alfa Bio, Banská Bystrica  
 VÚPOP Bratislava  
 Department of Biochemistry, University of Veterinary Medicine, Košice

### **B. International Cooperation:**

North Dakota State University, College of Pharmacy, Department of Pharmaceutical Sciences, Fargo, North Dakota, USA  
 - Subcellular pharmacokinetics; Prediction of the fate of xenobiotics in the environment  
 UFZ Centre for Environmental Research, Department of Chemical Ecotoxicology, Leipzig, Germany  
 - Degradation of pollutants in sediments  
 BCS Engineering, Brno, Czech Republic  
 -Bioconversion of maleinanehydride to organic acids  
 Mega a.s., Stráž pod Rálskem, Czech Republic  
 - Encapsulation of microorganisms to PVA Gel  
 Office International de la Vigne et du Vin, Paris, France  
 -Evaluation of wine  
 Agricultural University, Brno, Czech Republic  
 -Microbiology of wine fermentation  
 Wine Establishment, Znojmo - Šatov, Czech Republic  
 -Chemistry of red wine  
 Kyoto University, Department of Agricultural Chemistry, Kyoto, Japan  
 -Overproduction and regulation of microbial polyunsaturated fatty acids  
 National Institute of Advanced Science and Technology, Tsukuba, Japan  
 -Biochemistry and overproduction of microbial polyunsaturated fatty acids  
 Office International de la Vigne et du Vin, Paris, France  
 -In Wine Tasting Commission  
 Pure and Applied Biochemistry, University of Lund, Sweden  
 -Enzyme thermistor applications in analysis  
 Division of Biotechnology IFM, Linköpings Universitet Linköping, Sweden  
 -Development and application of biosensors

### **C. Membership in Domestic Organizations and Societies:**

Slovak Society of Biotechnology, Bratislava (J.Augustín, K.Dercová, D.Slugeň)  
 Slovak Society for Biochemistry and Molecular Biology, Bratislava (J.Augustín)  
 Slovak Society for Agriculture, Forestry, Food and Veterinary Sciences, Bratislava (J.Šajbidor, D.Slugeň)

### **D. Membership in International Organizations and Societies:**

Editorial boards of the journal Kvasný průmysl, Prague, Czech Republic (F.Malík, D.Šmogrovičová)  
 ECE Governments on Science and Technology of The United Nations, Geneva, Switzerland (J.Augustín)  
 Member of the EBC Brewing Science Group, Zoeterwoude, The Netherlands (D.Šmogrovičová)  
 Czecho-Slovak Society of Microbiology, Bratislava (J.Augustín, K.Dercová, D.Haláma, D.Šmogrovičová, M.Šturdíková)  
 SETAC-Society for environmental Toxicology and Chemistry (R.Tandlich)

### **E. CEEPUS PROGRAMME**

Number H-0115, Green Network in Central Europe (Šmogrovičová D., Dömény Z.) Coordinator: Szent Istvan University, Buda Campus (University of Horticulture and Food Industry)  
 University of Agriculture, Forestry and Renewable Natural Resources, Vienna  
 Mendel University of Agriculture and Forestry, Brno  
 University of Agriculture in Wrocław  
 University of Agriculture in Nitra  
 Josip Juraj Strossmayer University of Osijek  
 Slovak University of Technology in Bratislava  
 University of Ljubljana

### **G. Visitors from Abroad:**

Assoc.Prof.J.Čepička University of Chemical Technology, Prague, Czech Republic, December 2000 (2 days)



**H. Visits of Staff Members and PhD Students to Foreign Institutions:**

|                 |  |
|-----------------|--|
| M. Čertík       | Tomáškovy dny, Brno, Czech Republik, June 6-8, 2001 3 days   |
| K. Dercová      | Biodegradation, Seč u Chrudimi, Czech Republic, March 7-8, 2001 2 days   |
| K. Dercová      | ECB, 10 <sup>th</sup> European Congress on Biotechnology, Madrid, Spain, July 7-11, 2001 5 days  |
| Z. Dömény       | CEEPUS, Intensive Course Wine Technology and Biotechnology, Budapest, Hungary, April 22-29, 2001 7 days                                  |
| Z. Dömény       | 19th Malting and Brewing Days, October 24-26, 2001, Brno, Czech Republic 3 days  |
| F. Malík        | CEEPUS, Intensive Course Wine Technology and Biotechnology, Budapest, Hungary, April 22-29, 2001 7 days                                  |
| F. Malík        | Vinalies Paris, France, February 21-26, 2001, 6 days   |
| F. Malík        | II. Int. Winw Competition Thessaloniki, Greece, February-March 27-3, 2001, 5 days  |
| F. Malík        | 47. Vino Ljubljana, Slovenia, March 22-27, 2001, 6 days  |
| F. Malík        | Selection Mondiales Brussel, Belgium, April 7-11, 2001, 5 days   |
| F. Malík        | Prix Zarcillo, Valladolid, Spain, June 4-8, 2001, 5 days   |
| F. Malík        | 10 <sup>th</sup> Vinoforum Prag, Czech Republic, July 11-14, 2001, 4 days  |
| F. Malík        | Mundus Vini, Neustadt, Germany, September 7-9, 2001, 4 days  |
| F. Malík        | 26 <sup>th</sup> World Congress of Wine, Adelaide, Australia, October 9-18, 2001, 10 days  |
| M. Navrátil     | 19th Malting and Brewing Days, Brno, Czech Republic, October 24-26, 2001, 3 days   |
| M. Navrátil     | Linköping University, Sweden, August 13-15, 2001, 3 days   |
| H. Hronská      | Tomáškovy dny, Brno, Czech Republik, June 6-8, 2001, 3 days  |
| M. Rosenberg    | CPH 2000, Milano, Italia, November 7-11, 2001, 4 days,   |
| M. Rosenberg    | Vitafood, Geneva, Switzerland, April 24-27, 2001, 4 days   |
| D. Slugeň       | CEEPUS, Intensive Course Wine Technology and Biotechnology, Budapest, April 22-29, 2001, 7 days  |
| D. Šmogrovičová | EBC Congress, Budapest, Hungary, May 12-18, 2001, 7 days,  |
| D. Šmogrovičová | CEEPUS, J.J. Strossmayer University in Osijek, Osijek Croatia, June 12-22, 2001, 10 days   |
| D. Šmogrovičová | 19th Malting and Brewing Days, Brno, Czech Republic, October 24-26, 2001, 3 days   |
| J. Zígová       | Lausanne EPFL, Technical University, Switzerland, 2001, 1 year   |
| I. Voštiar      | Study state, Linköping University, Sweden, 1.10. 2001- 1.10.2002- 1 year   |
| I. Voštiar      | Tomáškovy dny, Brno, Czech Republik, June 6-8, 2001, 3 days  |
| L. Sláviková    | Tomáškovy dny, Brno, Czech Republik, June 6-8, 2001, 3 days  |
| R. Tandlich     | Study state, North Dakota State University, North Dakota, USA, 2001, 1 year  |
| M. Hazlingerová | King Technical Institute, Stokholm, Sweden 2000-2001 Sept.-Jan. 5 month  |
| D. Kóňová       | Dánsko ECCO SkoA/5, Bredebro – International Shoe Company, Jan.-Feb.2001 (Chemical Engineering Trainee, ECCO's Group Quality Department) |
| M. Rebroš       | University of Luton, Great Britain, 2001   |
| M. Pavlíková    | (CEEPUS, J.J. Strossmayer University in Osijek, Marz 2001  |
| K. Volleková    | (Szent István University, Faculty of Food Sciences, Budapest)CEEPUS, Marec 2001  |
| B. Raczová      | (Szent István University, Faculty of Food Sciences, Budapest, CEEPUS, Marec 2001   |

**VI. THESES AND DISSERTATIONS****A. Graduate Thesis (MS Degree) for state examinations after five years of study (supervisors are written in brackets):**

|                  |  |
|------------------|--|
| Baráthová Z.:    | Optimisation of ethanol fermentation with immobilised yeasts. (E. Šturdík)                       |
| Brnáková Z.:     | Azaphilone pigment production and isolation by the Monascus strains. (D. Slugeň)                 |
| Bugárová L.:     | Relationship between polyols formation and lipid biosynthesis in osmotolerant yeasts.(M. Čertík) |
| Gajdošíková E.:  | Enzymatic hydrolysis of starch substrates for ethanol fermentation.(E. Šturdík)                  |
| Hazlingerová M.: | Screening of compounds of natural origin with antiprotease activity. (T. Maliar)                 |
| Hranická S.:     | Xenobiotics degradation by microorganisms. (J. Augustín)   |

|                  |  |
|------------------|--|
| Jurčíková Z.:    | Microbial production of erythritol by the yeasts of the genus <i>Aureobasidium</i> and <i>Trichosporonoides</i> . (M. Rosenberg) |
| Juršíková P.:    | Protective role of polysaccharides in yeast cells for toxic effect of Cd <sup>2+</sup> and Ni <sup>2+</sup> ions. (M. Čertík)    |
| Klimko J.:       | Biotechnological aspects of secondary wine fermentation. (F. Malík)  |
| Kóňová D.:       | Production of yeast's beer with the microelements. (Z. Dömény)   |
| Matušiková M.:   | Preparation of tartaric acid by the immobilised cells <i>Nocardia</i> sp. CCM 4837/A. (H. Hronská)                               |
| Michalisková L.: | Primary biodegradation of xenobiotics. (J. Augustín)   |
| Mikušová L.:     | Analysis of volatile products of Italian Riesling. (J. Krupčík)  |
| Monošíková M.:   | Continuous production of beverages based on honey by immobilised yeast. (M. Navrátil)  |
| Mrňák R.:        | Biosensors for determination of glucose with immobilised glucose oxidase. (J. Tkáč)  |
| Pavlíková M.:    | Characterization of beer produced from very high gravity substrates using immobilised yeasts. (D. Šmogrovičová)                  |
| Pekarová T.:     | The influence of the immobilisation on yeast metabolism and fermentation in stress conditions. (D. Šmogrovičová)                 |
| Pigoš M.:        | Fungal inhibitors of the patho-physiological proteinases. (M. Šturdíková)  |
| Ráczová B.:      | Production of beverages with the help promoting effect. (Z. Dömény)  |
| Salugová D.:     | Microbial degradation of chlorinated phenols. (K. Dercová)   |
| Špániková S.:    | Effect of detergents on growth and lipid composition in <i>Trichoderma viride</i> . (M. Čertík)                                  |
| Tybitanclová K.: | Production of the cytotoxic metabolites by endophytic micromycetes. (M. Šturdíková)  |
| Valach M.:       | Biosensors for determination of ethanol with use of alcohol dehydrogenase. (J. Tkáč)   |
| Vargová K.:      | Development of fermented juices by yeast with defect in TCA cycle. (M. Navrátil)   |
| Volleková K.:    | Yeast strains of Slovak vine region Tokay. (F. Malík)  |

## B. Dissertations (PhD):

|              |  |
|--------------|--|
| Navrátil M.: | Innovations of fermentation processes using microorganisms immobilized in hydrogels. |
|--------------|--|

## VII. PUBLICATIONS

### A. Journals (\*registered in Current Contents)

- [1]\* Bagan S.G., Šmogrovičová D., Dömény Z., Stopka J., Schlosser Š.: Využitie „crossflow“ mikrofiltrácie v pivovarníctve. Application of the crossflow microfiltration in the brewing industry (in Slovak). *Kvasny Prum.* 47 (4), 97-101, (2001)
- [2] Čertík M.: Nihonshu - Japonské saké. 1. časť: História. *Vinohrad a Víno*, 1, 2001, 13-15. (Nihonshu – Japanese sake. 1. part: History (in Slovak). *Vinohrad a Víno*, 1, 13-15, 2001)
- [3] Čertík M.: Nihonshu - Japonské saké. 2. časť: Tajomstvo premeny ryže a vody na saké. *Nihonshu – Japanese sake. 2. part: Mystery of rice and water changing to sake (in Slovak). Vinič a Víno*, 1(3), 61-63, 2001
- [4] Furdíková K., Vollek V., Malík F.: Kvasinky slovenskej tokajskej vinohradníckej oblasti. 1. časť: Izolácia a charakterizácia potenciálnych kmeňov. *Yeasts of Slovak Tokay Wine Region. Part I. Isolation and characterisation of potencial strains (in Slovak). Vinič a víno* 1, No 6, 2,3,6 (2001)
- [5]\* Horváthová V., Janeček Š., Šturdík E.: Amylolytic enzymes: Molecular aspects of their properties. *General Physiology and Biophysics* 20, 7-32 (2001)
- [6] Horváthová V., Janeček Š., Šturdík E.: Štruktúra, stabilizácia a využitie amyláz. *Nova Biotechnologica* 1, 97-125 (2001)
- [7] Horváthová V., Šturdík E., Janeček Š.: Stabilita, stabilizácia a aplikácia amyláz. *Stability, stabilization and application of amylases (in Slovak). Bulletin of Food Research* 40, 1-20 (2001)
- [8] Kováčová S., Šturdík E.: Bioremediácia rádionuklidmi znečistených oblastí. *Nova Biotechnologica* 1, 51-65 (2001)
- [9]\* Lešová K., Šturdíková M., Proksa B., Pigoš M., Liptaj T.: OR-1-a mixture of esters of glyceric acid produced by *Penicillium funiculosum* and its antitrypsin activity. *Folia Microbiol.* 46 (1), 21-23 (2001)
- [10] Malík F.: Imobilizované vinne kvasinky. *Immobilized wine yeasts (in Slovak). Kvasny Prum.* 47,(9), 242 – 243, (2001)
- [11]\* Miková H., Rosenberg M., Krištofiková L.: Production of dicarboxylic acids important for technology. *Chemical papers* 95, 28-33, (2001)
- [12]\* Navrátil M., Šturdík E.: Batch and continuous mead production with pectate immobilized, ethanol-tolerant yeast. *Biotechnology Letters* 23, 977-982 (2001)
- [13]\* Navrátil M., Švitel J., Tkáč J., Danielsson B., Šturdík E.: Monitoring of the bioconversion of glycerol to dihydroxyacetone with immobilized *Gluconobacter oxydans* cells using thermometric flow injection analysis. *Process Biochemistry* 11, 7-14 (2001)
- [14] Oravcová K., Kačíková E., Šturdík E.: Metódy na rýchle odlišenie *Listeria monocytogenes* od ostatných baktérií. *Nova Biotechnologica* 1, 126-135 (2001)
- [15] Pátková J., Šmogrovičová D., Dömény Z., Bafrcová P.: Adaptácia voľných a imobilizovaných pivovarských kvasiniek pri skvasovaní vysoko koncentrovaných mladín. *Adaptation of free and immobilized brewery yeast during attenuation of highly concentrated hopped worts (in Slovak). Kvasny Prum.* 47 (1), 7-10, (2001)
- [16] Slugeň D.: Slovenské vína 2001 - bol to dobrý rok. *Slovak wines 2001 - it was a good year (in Slovak). Vinič a víno* 1, 6, 121 – 122 (2001)

- [17] Slugeň D.: Technológia a biotechnológia vína v strednej Európe. Wine technology and biotechnology in the Middle Europe (in Slovak). Vinič a víno 1, 3, add. 6 (2001)
- [18] Slugeň D.: Tisícročné víno. Thousand years wine (in Slovak). Kvasny Prum. 42, 9, 270 (2001)
- [19] Slugeň D.: Tokajské zlaté inžinierstvo. Tokay gold engineering (in Slovak). Vinič a víno 1, 5, add. 2,3,6 (2001)
- [20] Slugeň D.: V kraji červených vín najviac chutilo biele. In the landscape of red wines best tastes the white one (in Slovak). Vinič a víno, 1,4, add. 3,6,7 (2001)
- [21] Slugeň D.: Vi(n)zážisti. Wine imagemakers (in Slovak). Vinič a víno 1, 2, 25 – 26 (2001)
- [22]\* Šmogrovičová D., Dömény Z., Švitel J.: Modelling of saccharide utilization in primary beer fermentation with yeast immobilized in calcium alginate. Applied Biochemistry and Biotechnology. 94 (1) 147-158, (2001)
- [23]\* Tandlich R., Brežná B., Dercová K.: The effect of terpenes on the biodegradation of polychlorinated biphenyls by *Pseudomonas stutzeri*. Chemosphere 44, 1547-1555 (2001)
- [24]\* Tkáč J., Navrátil M., Šturdík E., Gemeiner P.: Monitoring of dihydroxyacetone production during oxidation of glycerol by immobilized *Gluconobacter oxydans* cells with an enzyme thermistor. Enzyme and Microbial Technology 28, 383-388 (2001)
- [25]\* Tkáč J., Voštiar I., Šturdík E., Gemeiner P., Mastihuba V. and Annus J.: Fructose biosensor based on D-fructose dehydrogenase immobilised on ferrocene embedded cellulose acetate membrane. Analytica Chimica Acta 439, 39-46 (2001)

## B. Conferences (\*international conferences)

- [1]\* Čertík M., Breierová E., Juršíková P., Šajbidor J.: Lipid structural changes of yeasts grown under heavy metal presence. Proceedings of XXIX. International Conference of Yeasts, Smolenice, 2001, p. 68
- [2]\* Čertík M., Breierová E., Šimončíková P., Šajbidor J.: Characterization of yeast lipids affected by salt stress. Proceedings of XXIX. International Conference of Yeasts, Smolenice, 2001, p. 67
- [3]\* Čertík M., Bugárová L., Krištofiková L., Rosenberg M.: Štruktúrne zmeny lipidov u kvasiniek tvoriacich polyoly. Structural changes of lipids from yeasts producing polyols (in Slovak). Proceedings of 22. International Congress of the Czechoslovak Society for Microbiology "Health and Microorganisms", Košice, 2001, p. 135
- [4]\* Čertík M.: Využitie chromatografických metód pri sledovaní mikrobiálnej syntézy mastných kyselín. The use of chromatographic methods for determination of microbial fatty acids synthesis (In Slovak). Proceedings of XIII. International Conference LABORALIM, Banská Bystrica, 2001, p. 87-90 (ISBN 80-227-1524-7)
- [5]\* Čertík M.: Extrakcie mikrobiálnych lipidov klasickými metódami a superkritickým CO<sub>2</sub>. Extraction of microbial lipids by classical methods and supercritical CO<sub>2</sub> (In Slovak). Proceedings of XIII. International Conference LABORALIM, Banská Bystrica, 2001, p. 268-276 (ISBN 80-227-1524-7)
- [6]\* Čertík M.: Physiological regulation of lipid biosynthesis in yeasts. Proceedings of XXIX. International Conference of Yeasts, Smolenice, 2001, p. 22
- [7]\* Dercová K.: Biodegradácia PCB a možnosti zvyšovania jej účinnosti. Biodegradation of PCBs and some possibilities of its enhancement (in Slovak). In: Book of Abstracts Biodegradation conference V. (O. Halousková, ed.), Seč, Czech Republic, March 7-8. 2001 p. 37-43.
- [8]\* Dercová K.: Biodegradation of PCBs and induction of their cometabolism. 10<sup>th</sup> European Congress on Biotechnology. In: Abstract Book, ENV 21, Madrid (Spain), July 8-11, 2001, p. 126
- [9]\* Dercová K., Kyselová Z., Salugová D., Barančíková G.: Biodegradácia pentachlórfenolu (PCP). Biodegradation of pentachlorophenol (PCP) (in Slovak). 22<sup>nd</sup> International Congress of the Czechoslovak Society for Microbiology Health and Microorganisms. In: Book of Abstracts, Košice 2001, p. 141
- [10]\* Dercová K., Tandlich R., Brežná B.: Vplyv terpenov na biodegradáciu polychlórovaných bifenylov (PCB). The effect of terpenes on biodegradation of PCBs (in Slovak). 22<sup>nd</sup> International Congress of the Czechoslovak Society for Microbiology Health and Microorganisms. In: Book of Abstracts, Košice 2001, p.39
- [11]\* Dömény Z., Ráczová B., Navrátil M., Šmogrovičová D., Šturdík E.: Vplyv teploty fermentácie na tvorbu senzorycky aktívnych látok pri výrobe medoviny pomocou imobilizovaných buniek. The influence of fermentation temperature on sensoric products formation during fermented honey production using immobilized cells (in Slovak). XIII. International Conference LABORALIM. In: Abstracts book Laboralim 2001, Banská Bystrica, February 7-8, 2001 p. 95-98
- [12]\* Dömény Z., Šmogrovičová D.: Degradácia  $\alpha$ -acetolaktátu imobilizovanou  $\alpha$ -acetolaktátdekarboxylázou.  $\alpha$ -Acetolactate degradation using immobilised  $\alpha$ -acetolactate decarboxylase (in Slovak). 19th Day of brewing and malting. In: Abstracts of lectures and posters Brno, October 25-26, 2001, p. 13.
- [13]\* Horváthová V., Šturdík E.: Utilisation of amylolytic enzymes for preparation of starch hydrolyzates for ethanol fermentation, Structure and Stability of Biomacromolecules SSB 2001. In: Book of Abstracts, Košice, September 12-14. 2001, p. 95-96
- [14]\* Horváthová V., Navrátil M., Šturdík E.: Hydrolysis of starch substrates by amylases before fermentation. The First Symposium on the Alpha-Amylase Family. In: Book of Abstracts, Smolenice, September 30. - October 4. 2001, p. 116
- [15]\* Hronská H., Rosenberg M., Krištofiková L.: Maleic acid anhydride as biotechnological material. XIII. International conference about analytical methods in food industry LABORALIM 2001. In: Book of Abstracts Laboralim 2001, Banská Bystrica, February 7.-8. 2001, p. 114-116.
- [16]\* Hronská H., Rosenberg M., Krištofiková L.: The use of yeasts for malic acid production. 22<sup>nd</sup> Congress of Czechoslovak Society for Microbiology with international participation on the topic of "Health and Microorganisms". In: Book of Abstracts Košice, Slovak republic, September 5.-9. 2001, p. 176.
- [17]\* Hronská H., Rosenberg M., Krištofiková L.: Microbial production of tartaric acid. Conference of the Young Microbiologists, Tomáškovy dny 2001. In: Book of Abstracts Brno, Czech Republic, June 6.-8. 2001, p. 13.
- [18] Koreňová A., Uher M., Milovník P., Šturdíková M.: Inactivation of the esterase activity by some derivatives of kojic acid. Abstract Book of the 53th Congress of Chemical Societies, Banská Bystrica 2001, p. 196-197 (ISBN 80-89029-24-8)
- [19]\* Kováčová S., Lesný J., Šturdík E.: Biotechnologies in nuclear waste management, Proceedings of II. Conference of Environmental Science, Széchenyi István University. In: Book of Abstracts, Győr, Hungary, p. 95-104
- [20]\* Krištofiková L., Rosenberg M., Hronská H.: Production of erythritol by various species of osmophilic yeasts. 22<sup>nd</sup> Congress of Czechoslovak Society for Microbiology with international participation on the topic of "Health and Microorganisms". In: Book of Abstracts Košice, Slovak republic, September 5.-9. 2001, p. 219.

- [21]\* Krištofiková L., Rosenberg M., Hronská H.: Formation of polyunsaturated fatty acids during lactic acid production by *Rhizopus* sp. XIII. International conference about analytical methods in food industry LABORALIM 2001. In: Book of Abstracts Laboralim 2001, Banská Bystrica, February 7.-8. 2001, p. 152-155.
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### II. TEACHING AND RESEARCH LABORATORIES

Laboratory of Animal Cell Cultures  
Laboratory of Biochemistry of Cancer Cells  
Laboratory of Fungal Biochemistry and Physiology  
Laboratory of Immunochemistry  
Laboratory of Microbiology

### III. TEACHING

#### A. Undergraduate Study

**1st semester (autumn)**

|                                 |         |  |
|---------------------------------|---------|--|
| Biology                         | (2-0 h) | Jantová, Horáková, Mikulášová                      |
| Laboratory Practices in Biology | (0-1 h) | Jantová, Dudová, Šovčíková, Poturnajová, Kaiserová |

**3rd semester (autumn)**

|  |         |  |
|--|---------|--|
| Microbiology I                         | (2-0 h) | Hudecová                                       |
| Laboratory Practices in Microbiology I | (0-2 h) | Hudecová, Majtán*, Mikulášová, Dudová, Pokorný |

**4th semester (spring)**

|  |         |   |
|--|---------|---|
| Biochemistry I                         | (2-0 h) | Varečka   |
| Laboratory Practices in Biochemistry I | (0-2 h) | Varečka, Paulíková, Chovanec, Lakatoš, Kaiserová, Pokorný |

**5th semester (autumn)**

|                               |         |      |
|-------------------------------|---------|------|
| Principles of Human Nutrition | (2-0 h) | Miko |
|-------------------------------|---------|------|

**6th semester (spring)**

|                    |         |  |
|--------------------|---------|--|
| Laboratory Project | (0-4 h) | Miko, Horáková, Varečka, Hudecová, Jantová, Mikulášová, Majtán*, Dudová, Pokorný |
|--------------------|---------|--|

**7th semester (autumn)**

|   |         |                                       |
|---|---------|---------------------------------------|
| Biochemistry II                         | (2-0 h) | Varečka                               |
| Laboratory Practices in Biochemistry II | (0-2 h) | Paulíková, Chovanec, Lakatoš, Hudec   |
| Microbiology II                         | (2-0 h) | Mikulášová, Hudecová                  |
| Laboratory Practices in Microbiology II | (0-2 h) | Hudecová, Majtán*, Mikulášová, Dudová |
| Immunochemistry                         | (2-0 h) | Ferenčík*                             |
| Seminar in Immunochemistry              | (0-1 h) | Ferenčík*                             |
| Laboratory Practice in Immunochemistry  | (0-2 h) | Daussant*, Kaiserová, Hudec, Kaliňák  |
| Biosensors                              | (2-0 h) | Labuda*                               |
| Biosensor Seminar                       | (0-1 h) | Labuda*                               |
| Biosensors Laboratory Practices         | (0-2 h) | Labuda*                               |

**8th semester (spring)**

|   |         |  |
|---|---------|--|
| Molecular Biology and Genetics  | (2-0 h) | Mikulášová, Paulíková  |
| Applied Microbiology  | (2-0 h) | Hudecová, Majtán*  |
| Bioenergetics   | (2-0 h) | Miko   |
| Laboratory Practices in Bioenergetics   | (0-2 h) | Miko   |
| Mechanisms of Action of Natural Compounds   | (2-0 h) | Varečka  |
| Mechanisms of Action of Natural Compounds<br>-Laboratory Practices                          | (0-2 h) | Dudová, Pokorný  |
| Laboratory Practices of the branch Biomedical<br>Engineering, Biochemistry and Microbiology | (0-4 h) | Miko, Horáková, Varečka, Hudecová, Jantová,<br>Mikulášová, Majtán* |

**9th semester (autumn)**

|   |           |  |
|---|-----------|--|
| Genetic Manipulations   | (2-0-2 h) | Čertík*  |
| Clinical Biochemistry   | (2-0 h)   | Chandoga*  |
| Clinical Biochemistry-Laboratory Practices  | (0-2 h)   | Chandoga*  |
| Cell cultures   | (2-0 h)   | Jantová, Horáková  |
| Laboratory Practices of the branch Biomedical<br>Engineering, Biochemistry and Microbiology | (0-6 h)   | Horáková, Hudecová, Jantová, Miko,<br>Mikulášová, Varečka, Majtán* |

**10th semester (spring)**

|                         |          |  |
|-------------------------|----------|--|
| Master's Thesis Seminar | (3-0 h)  | Miko, Horáková, Varečka, Hudecová, Majtán* |
| Master's Thesis         | (0-27 h) | Miko, Horáková, Varečka, Hudecová, Majtán* |

**B. PhD Study**

|                    |                    |
|--------------------|--------------------|
| Biochemistry       | Miko, Varečka      |
| Microbiology       | Horáková, Hudecová |
| *-external teacher |                    |

**VI. CURRENT RESEARCH PROJECTS****A. Cytotoxicity of novel xenobiotics and their mode of action (Milan Miko)**

The primary aim of our group is the identification and evaluation of potential anti-cancer agents. The main results are as follows:

1. Fourteen substituted 4-anilinoquinazolines, seventeen plant extracts and four preservative compounds for cosmetics were tested for cytostatic, genotoxic, anticancer and antibacterial effects. The most active 4-anilinoquinazolines were substituted by chlorine or bromine group in the aromatic ring, in the pyrimidine ring by morpholine group and in the aniline skeleton by nitro group in position 4 or 2. Four anilinoquinazolines inhibited growth of tumor cell lines HeLa, B16 and L1210 and exhibited antiprotease effect on plasmin. Concentration 5.2  $\mu\text{mol/L}$  of 6-bromo-2-(morpholin-1-yl)-4-anilinoquinazolinone induced a significant increase of filamentous actin in the transformed HepG2 cells. A 35 % degradation of HeLa cells was found after 72 h treatment with 62.5  $\mu\text{g/mL}$  of the extract isolated from *Stephanandra tanakae*. The 100 % lysis of HeLa cells was observed after 72 h treatment by 125  $\mu\text{g/mL}$  concentration of the extract prepared from *Gymnocladus dioicus*. The extracts from *Ligustrum devayanum* and *Ligustrum vulgare* are specifically effective only with HeLa cells. On the other hand, the extract prepared from *Gymnocladus dioicus* is effective on the bacteria and on the HeLa cells too. Preservative Bronopol demonstrated the highest cytotoxic effect on the proliferation of V79 and VH10 fibroblast cell lines.

2. In the frame of mode of action of 8 novel isothiocyanate derivatives (ITCs) was found out, that two carcinoma cell lines (A2780, A431) appeared extremely sensitive to the majority of the tested ITCs ( $\text{ID}_{50} = 2.2\text{--}8.0 \mu\text{mol/l}$ ). The tested ITCs modified the cell cycle of carcinoma cell lines (A2780, A2780/ADR, A431) and sarcoma cell lines (B-5GT, BP6-TU2), as well as leukemic cell line (JURKAT), mainly at 10  $\mu\text{mol/l}$  and 5  $\mu\text{mol/l}$ . The gradual inhibition of cell proliferation was observed, characterised by decreasing of percentage of cells in  $G_0/G_1$  phase and accumulation of cells in S and  $G_2/M$  phases of the cell cycle. Four from the five tested ITC derivatives showed the ability of strong induction of apoptosis (34-27%) in A2780 carcinoma cells.

3. Four trisubstituted quinazolinone derivatives exerted a significant effect on *E. coli*, *P. aeruginosa*, *S. aureus* and *B. subtilis* ( $\text{IC}_{50} < 100 \text{ mg/l}$ ) and influenced the specific growth rate. The results of primary screening for cytotoxicity of eighteen plant extracts showed that the extracts which have manifested 100% toxicity on HeLa cells come from the family Fabaceae, Rosaceae, Oleaceae and Staphyleaceae. The cytotoxically effective extracts represent three different types of cytotoxic effect – acute, delayed and combined effect. The effect of Cu tetraaza macrocyclic complex on the glutathione status was examined and the possible mechanism of this anticancer-membrane targeting drug was studied. In the frame of genotoxic effects of Cu(II) complexes of mephenamate, flufenamate, acetylsalicylate was found that these compounds statistically significantly decreased the number of revertants induced by 2-aminoanthracene and 2-aminofluorene. This antimutagenic activity is associated with the copper properties to participate in a number of different biological processes and its interaction with DNA. The genotoxic effects of lignin and selected degradation products of lignin were studied.

**B. Biochemical processes underlying fungal differentiation and secondary metabolism (Ludovít Varečka)**

In the project devoted to study the transport processes in filamentous fungi several aspects of transport and physiology were studied.

In *Trichoderma viride* the process of chloride transport was studied by means of  $^{36}\text{Cl}$  radionuclide. It was found that chloride anions enter the vegetative mycelia in a saturable, pH- and temperature-dependent manner with selectivity for chlorides and bromides. Further properties of transport suggest that chloride anions are transported by a specific and electrically silent transport



protein. In *Penicillium simplicissimum* the process of citrate transport into the vegetative mycelia has been described and the conditions were found which led to the induction of novel citrate uptake system driven by protonmotive force. Its role in the citrate metabolism is being currently analysed.

In the project devoted to study the conidiation and physiology of filamentous fungi, the physiology of development and conidiation has been studied. It was found that the conidiation of *Trichoderma* observed in the dark is induced neither by starvation nor steric constraints and probably could be related to the genetical program of the organism. This notion could be supported by the isolation of mutants with delayed conidiation but normal growth characteristics. Further, the changes of the energy metabolism were studied in the submerged mycelia which revealed a strong dependence of various parameters (respiration, citrate production, etc.) on the developmental status which complement our previous data concerning the  $Ca^{2+}$  uptake or glutamate decarboxylase activity and suggest that there rate of metabolism is a function of developmental stage of mycelia.

## V. COOPERATION

### A. Cooperation in Slovakia

Institute of Chemistry, Slovak Academy of Sciences, Bratislava  
 Institute of Animal Physiology and Biochemistry, Slovak Academy of Sciences, Bratislava  
 Institute of Molecular Physiology, Slovak Academy of Sciences, Bratislava  
 Institute of Animal Biochemistry and Genetics, Slovak Academy of Sciences, Ivánka pri Dunaji  
 Cancer Research Institute, Slovak Academy of Sciences, Bratislava  
 Faculty of Pharmacy, Comenius University, Bratislava  
 Faculty of Natural Sciences, Comenius University, Bratislava  
 Institute of Preventive and Clinical Medicine, Bratislava  
 Institute of Virology, Slovak Academy of Sciences, Bratislava  
 Dairy Research Institute, Žilina  
 Department of Chemistry, Paedagogical Faculty, University, Trnava  
 Department of Medical Chemistry, Biochemistry and Clinical Biochemistry, Faculty of Medicine, Comenius University, Bratislava  
 Department of Molecular Biology, Faculty of Natural Sciences, Comenius University, Bratislava  
 Institute of Immunology, Faculty of Medicine, Comenius University, Bratislava

### B. International Cooperation:

Laboratoire du Biomembranes et Messagers Cellulaires, Université Paris XI, Orsay, France (Dr. Françoise Giraud)  
 Laboratory of Cell Signalling, Nagoya University Bioscience Center, Nagoya, Japan (Prof. Dr. Shoshi Toriyama)  
 Institut für Mikrobiologie, Universität zu Innsbruck, Innsbruck, Austria (Prof. Dr. Wolfgang Burgstaller)  
 Botanisches Institut, Friedrich Wilhelms Universität, Bonn, Germany (Dr. Udo Hoelker)  
 ReaD VUFB, a.s. Prague, Czech Republic  
 Liverpool John Moores University, Liverpool, UK  
 - Electron microscopy of photo-induced conidiation and dimorphism in Fungi.  
 Université de Genève, Genève, Suisse  
 - Biochemistry and molecular biology of photo-induced conidiation in Fungi.  
 European Organisation on Research and Treatment of Cancer, Screening and Pharmacology Group, University of Tokushima, Japan  
 - Uncouplers of oxidative phosphorylation.  
 Institute of Food Research, Norwich, UK  
 - Rapid, specific detection of *Listeria monocytogenes* by antibody-based techniques and on-line sensor technology.  
 Institute of Chemical Technology, Prague, Czech Republic  
 - Rapid, specific detection of *Listeria monocytogenes* by antibody-based techniques and on-line sensor technology.  
 MILCOM a.s., Dairy Research Institute, Prague, Czech Republic  
 - Rapid, specific detection of *Listeria monocytogenes* by antibody-based techniques and on-line sensor technology.  
 Dublin City University, Dublin, Ireland  
 - Rapid, specific detection of *Listeria monocytogenes* by antibody-based techniques and on-line sensor technology.

### C. Membership in Domestic Organizations and Societies:

|   |   |
|---|---|
| Slovak Society for Biochemistry and Molecular Biology, Bratislava | (M. Miko, L. Varečka)                     |
| Slovak Medical Society, Bratislava                                | (S. Jantová)                              |
| Czecho-Slovak Society for Biochemistry, Bratislava                | (S. Jantová)                              |
| Czecho-Slovak Society for Microbiology, Bratislava                | (K. Horáková, D. Hudecová, M. Mikulášová) |
| Czecho-Slovak Society for Biology, Brno                           | (K. Horáková, S. Jantová, M. Mikulášová)  |
| Oncological Society of the Slovak Medical Society, Bratislava     | (K. Horáková)                             |

### D. Membership in International Organizations and Societies:

|   |  |
|---|--|
| International Society for the Study of Xenobiotics, Bethesda, MD, U.S.A.            | (M. Miko)  |
| European Association for Cancer Research, Nottingham, U.K.                          | (M. Miko)  |
| European Organisation on Research and Treatment of Cancer, Moerkapelle, Netherland. | (M. Miko)  |
| European Tissue Culture Society   | (K. Horáková)  |
| EUROTOX-European Societies of Toxicology, Turku, Finland                            | (K. Horáková, S. Jantová, M. Mikulášová, A. Šovčíková) |

### F. International Scientific Programmes:

#### 1. INCO COPERNICUS

a) project PL 979012, „Rapid, specific detection of *Listeria monocytogenes* by antibody-based techniques and on-line sensor

technology., (K. Horáková)  
contract No. ERB IC15-CT98-0902 (1999-2001)  
Participating organizations:

Institute of Chemical Technology, Prague (CZ)  
Institute of Food Research, Norwich (UK)  
Slovak Univerzity of Technology, Bratislava (SK)  
Dublin City University, Dublin (I)  
MILCOM a.s., Dairy Research Institute, Prague (CZ)  
Dairy Research Institute, Žilina (SK)

### G. Visitors from Abroad:

Prof. Dr. Jean Daussant

C.N.R.S., Meudon, France, November 2001 (10 days)

### H. Visits of Staff Members and PhD Students to Foreign Institutions:

M. Kaliňák  
R. Pokorný  
B. Dudová

Universität Innsbruck, Innsbruck, Austria (90 days)  
Friedrich Wilhelms Universität, Bonn, Germany (90 days)  
XXIst Xenobiochemical symposium. Dolní Věstonice (Czech Republic), May-June 2001 (2 days)

M. Miko

XXIst Xenobiochemical symposium. Dolní Věstonice (Czech Republic), May-June 2001 (2 days)

## VI THESES AND DISSERTATIONS

### A. Graduate These (MS Degree) for state examinations after five years of study (supervisors are written in brackets external supervisors):

Cariková S.: Screening and mode of cytotoxic action of chosen xenobiotics. (M. Miko)

Čavojcová M.: Cytotoxicity and apoptotic potential of selected isothiocyanate derivatives. (K. Horáková)

Dudíková J.: Bioactive polypropylene fibres on the basis of Irgasan. (D. Hudecová)

Furjészová K.: Identification of virulence markers of *Salmonella enteritidis* strains isolated from food and clinical samples. (V. Majtán\*)

Horváth V.: Biological effects of some quinazoline derivatives. (S. Jantová)

Hudec R.: Using immunochemical and chromatography methods in calcium transport study in human red blood cells. (L. Varečka)

Kaliňák M.: Transport of the citric acid into the mycelia of *Penicillium simplicissimum*. (L. Varečka)

Kamenistá A.: Characterization of chlorpromazine-resistant *Trichoderma viride* mutants. (D. Hudecová)

Kamodyová M.: Optimalization of two-plasmid system for identification of promoters controlled by RNA-polymerase containing stress factor  $\delta^E$ . (J. Kormanec\*)

Krabáč B.: The influence of mineral fibrous dust on mammalian immune system. (J. Tulinská\*)

Lábaj J.: The role of lignin in reduction of genotoxic damage of mammalian cells. (D. Slameňová\*)

Luptáková I.: Aging of *Trichoderma viride* grown up in the submerged and surface cultivation. (L. Varečka)

Luptovcová M.: Modulation of glutathione metabolism and chemotherapy. (H. Paulíková)

Mellenová H.: Effect of new bisquaternary ammonium salts on *Stenotrophomonas maltophilia*. (V. Majtán\*)

Rolková G.: Genotoxic and antimicrobial activity of selected derivatives of quinazolines. (M. Mikulášová)

Teplická J.: The study of different types of lignin considering to their antimicrobial and genotoxic effects. (M. Mikulášová)

Trutzová R.: Immunochemical detection of the pathological forms of tau protein in the brain of the patient with Alzheimer disease. (E. Kontseková\*)

-\*external teacher

### B. Dissertations (PhD):

Chovanec P.: Metabolic aspect of vegetative growth and conidiation of *Trichoderma viride*. (L. Varečka)

Strigáčová J.: Antimicrobial (biological) activity of selected synthetic or natural compounds. (D. Hudecová)

Šovčíková A.: Antimicrobial activity and the mode of action of isothiocyanate derivatives. (K. Horáková)

### D. Habilitation Theses:

Jantová S.: Cytotoxicity, antimicrobial activity and the mechanism of effect of the

natural and synthetic compounds.

## VII PUBLICATIONS

### A. Journals (\*registered in Current Contents)

- [1] Brtko J., Hudecová D., Bransová-Bobálová J., Novotný L., Eybl V., Melník M., Uher M.: Kojic acid: a superior source for preparation of biologically active compounds (current experience). *Biomarkers Environment* 4, 26-30, (2001).
- [2]\* Dudová B., Hudecová D., Pokorný R., Mikulášová M., Palicová M., Segľa P., Melník M.: Copper complexes with bioactive ligands and their biological activity. *Folia Microbiol.* 46 (5), 379-384, (2001).
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- [4]\* Hojerová J., Jantová S., Hanusová B., Vollek V.: Antimicrobial efficacy of some interesting preservatives for cosmetics. *SOFW-Journal* 8, 9-15 (2001)
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- [7]\* Jantová S., Nagy M., Růžeková L., Grančai D. Cytotoxic effects of plant extracts from the families Fabaceae, Oleaceae, Philadelphaceae, Rosaceae and Staphyleaceae. *Phytother.Res.* 15, 22-25 (2001)
- [8]\* Jantová S., Urbančíková M., Maliar T., Mikulášová M., Rauko P., Čipák L., Kubíková J., Stankovský Š., Špirková K. Biological activity of some 4-anilinoguanazolines: cytotoxic, genotoxic and antiprotease effects, induction of necrosis and changes of actin cytoskeleton. *Neoplasma*, 48 (1), 52-60 (2001)
- [9]\* Jantová S.: Stratégia vyhľadávania nových látok účinných proti mikróbnym a nádorovým bunkám. The strategy of seeking of new compound effected against microbial and cancer cells. *Skripta Med.* 2, 130-131 (2001)
- [10] Jantová S., Hojerová J., Hanusová B., Mikulášová M.: Cytotoxická a genotoxická aktivita vybraných konzervačných látok pre kozmetické prostriedky. Cytotoxic and genotoxic activity of certain preservative agents in cosmetics (in Slovak) *Česká a slovenská farmacie*, 5, 238-242 (2001)
- [11]\* Koman M., Moncol J., Hudecová D., Dudová B., Melník M., Korabik, M., Mroziński J.: Copper(II) pyridine-2,6-dicarboxylates. Coordination and distortion isomers of [Cu(pydc)(H<sub>2</sub>O)<sub>2</sub>]. *Polish J. Chem.* 75, 957-964, (2001).
- [12]\* Košíková B., Alexy P., Mikulášová M., Kačík F.: Characterization of biodegradability of lignin-polyethylene blends. *Wood research* 46 (1), 31-36 (2001)
- [13]\* Mikulášová M., Košíková B.: Effect of blending lignin biopolymer on biodegradability of polyolefin plastics. *World Journal of Microbiology and Biotechnology* 17(6), 601-607 (2001)
- [14]\* Miko M., Turňa J., Stuchlík S., Souček R.: Oracine a novel inhibitor of topoisomerases I and II. 12th Mediterranean Congress of Chemotherapy, Morocco, November 11-14, 2001. Ed. H.Himmich. Monduzi Editore, Bologna, Italy, p.331-338
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- [17] Strigáčová J., Hudecová D.: Metodické aspekty stanovenia antimikrobiálnej aktivity. Methodical aspects of the assessment of antimicrobial activity (in Slovak). *Biologické listy* 66 (2), 113-124, (2001).
- [18]\* Sulo P., Hudecová D., Properová A., Bašňák I., Sedláček I.: 2,5-Diketo-D-gluconate production by a mixed culture of two newly-isolated strains: *Flavimonas oryzihabitans* and *Pseudomonas cepacia*. *Biotechnol. Lett.* 23, 693-696, (2001).
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### B. Conferences (\*international conferences)

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- [4]\* Horáková K., Greifová M., Seemanová Z., Gondová B., Wyatt G.M.: A microplate method for monitoring of *Listeria monocytogenes* growth kinetics and the influence on the expression of p60 in selected enrichment media. In: VI<sup>th</sup> International Conference on Agri-Food Antibodies, Prague 2<sup>nd</sup>-5<sup>th</sup> October 2001, Czech Republic, p.75 (Po)
- [5] Horáková K., Greifová M., Seemanová Z., Gondová B., Wyatt G.M.: Development of a microplate method for characterization of *Listeria* species growth kinetics and the influence of selected media on p60 expression. In: 22nd Congress of the Czechoslovak Society for Microbiology – Health and Microorganisms, Košice (Slovakia), 5<sup>th</sup>-9<sup>th</sup> september 2001, p.174 (Po)
- [6] Hudecová D., Dudová B., Valent A.: Antimikrobiálna aktivita Cu(II) komplexov s N-donorovými ligandami. Antimicrobial activity of Cu(II) complexes with N-donor ligands (in Slovak). In: 22nd Congress of the Czechoslovak Society for Microbiology - Health and Microorganisms, Košice (Slovak Republic), Sept. 5-9, 2001, p. 179. (Pr)

- [7] Hudecová D., Marcinčin A., Augustín J.: Bioaktívne textilné vlákna na báze Irgasanu. Bioactive textile fibres on the base of Irgasene (in Slovak). In: 22nd Congress of the Czechoslovak Society for Microbiology - Health and Microorganisms, Košice (Slovak Republic), Sept. 5-9, 2001, p. 47. (Pr)
- [8] Hudecová D., Strigáčová J., Dudová B.: Biologické účinky novosyntetizovaných derivátov chinolínu. Biological effects of new synthesised derivatives of quinine (in Slovak). In: 22nd Congress of the Czechoslovak Society for Microbiology - Health and Microorganisms, Košice (Slovak Republic), Sept. 5-9, 2001, p. 180. (Pr)
- [9]\* Hudecová D., Dudová B., Uher M.: Tiomočovínové arylfuránové deriváty a ich antimikróbna účinnosť. Thiourea arylfuranol derivatives and their antimicrobial activity (in Slovak). In: XXIst Xenobiochemical symposium. Dolní Věstonice (Czech Republic), May 30 - Jun 1, 2001, p. 59. (Po)
- [10] Hudecová D., Uher M., Koreňová A., Melník M., Brtko J.: Deriváty kyseliny kojovej - perspektívny zdroj bioaktívnych zlúčenín využívatel'ných v ochrane rastlín. Derivatives of kojic acid - perspective source of bioactive compounds applicable in plant protection (in Slovak). In: 53rd Congress of Chemical Societies. Banská Bystrica (Slovakia), Sept. 3-6, 2000, I-PO22, p. 198-199. (Po)
- [11] Chovanec P., Liptaj T., Prónayová N., Varečka L.: Rast a metabolizmus *Trichoderma viride* pri obmedzenej dostupnosti kyslíka. The growth and metabolism of *Trichoderma viride* in limited oxygen conditions (in Slovak). Drobnicov memoriál, Smolenice (Slovak Republic), 8.-9.11. 2001, s.54-55
- [12]\* Hojerová J., Jantová S., Kandárová H.: Verification of the fibroblast cell lines for the toxicity testing of cosmetics. In: Abstracts of International Symposium on Promotion of the Three Rs Concept in Reaction to Animal Experimentation in Slovakia, Slovenia and the Czech Republic, Prague (Czech Republic), June 4-6 (2001) ISBN: 80-86313-05-0 (PPr)
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- [14]\* Jantová S., Slameňová D., Čipák L., Horváth V.: Biological activity of 9-bromo-5-morpholino-tetrazolo[1,5-c]quinazoline. In: Abstracts of XVI. Biologické dny Olomouc (Czech Republic), 5. - 7.9., p.117 (2001) ISBN 80-244-0327-7 (Po)
- [15]\* Karamonová L., Rauch P., Wyatt G.M., Greifová M., Horáková K.: Production of antibodies to *Listeria virulence* proteins and development of an ELISA for *L. monocytogenes*. In: VI<sup>th</sup> International Conference on Agri-Food Antibodies, Prague 2<sup>nd</sup>-5<sup>th</sup> October 2001, Czech Republic, p.115, (Po)
- [16] Karasová L., Greifová M., Novák P., Horáková K., Rauch P., Wyatt G.M.: The influence of media on immunochemical detection of *Listeria monocytogenes* cells. In: XXXII<sup>nd</sup> Symposium about new directions of production and valuation of food-stuffs. 28.-30.5.2001, Skalský Dvur (Czech Republic), p. 32, (Po)
- [17]\* Koman M., Melník M., Hudecová D., Moncol J., Dudová B., Glowiak T.: Crystal structure of copper(II) clofibrates with some derivatives of pyridine and their biological activity. In: Challenges for Coordination Chemistry in the New Century. Smolenice (Slovak Republic), Jun 4-8, 2001. Eds. Melník M., Sirota A., p. 71-76 (2001). ISBN 80-227-1539-5. (Po)
- [18]\* Košíková B., Sláviková E., Mikulášová M., Majerová B.: Biopulping of spruce wood by *Sporobolomyces roseus* and *Geotrichum klebahnii*. In: Proceedings of 11th International Symposium on Wood and Pulping Chemistry. Nice, France, June 11-14. 2001, pp.18-21(2001) (Po)
- [19]\* Košíková B., Kačík F., Alexy P., Mikulášová M.: Spectral and molecular characteristics of fractions isolated from biodegraded polyethylene containing lignin derived from chemical wood treatment. II. Miedzynarodowa konferencja naukowa Metody badan v chemicznej technologii drewna na przelomie wiekow. Zielonka k/Poznania, Pol'sko, Oct.18-20. 2001,
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- [27] Pokorný R., Strigáčová J., Hudecová D., Varečka L.: Zmeny aktivity GAD počas vývoja mycélia *Trichoderma viride* a ich regulácia. Changes in GAD activity during development of mycelia *Trichoderma viride* and their regulation.(In slovak). Drobnicov memoriál, Smolenice (Slovak Republic), 8.-9.11. 2001, p.72-73
- [28] Segla P., Palicová M., Dudová B., Hudecová D., Melník M.: Synthesis, spectral properties and antimicrobial effects of copper(II) pyridinecarboxylate adducts with N-hetero-cyclic ligands. In: Challenges for Coordination Chemistry in the New Century. Smolenice (Slovak Republic), Jun 4-8, 2001. Eds. Melník M., Sirota A., p. 245-250 (2001). ISBN 80-227-1539-5. (Po)
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- antimicrobial effects. In: Challenges for Coordination Chemistry in the New Century. Smolenice (Slovak Republic), Jun 4-8, 2001. Eds. Melník M., Sirota A., p. 251-256 (2001). ISBN 80-227-1539-5. (Po)
- [30] Sláviková E., Košíková B., Mikulášová M.: Biodegradation of waste lignin products by soil - inhabiting yeast organism. XXIXth annual conference on yeast. SAS Congres Centre Smolenice (Slovak Republic), May 23-25, 2001 (Po)
- [31] Šovčíková A., Mikulášová M., Horáková K.: Štúdium mutagénnych a cytotoxických účinkov izotiokyanátov. The study of mutagenic and genotoxic effects of isothiocyanates (in Slovak). In: 22nd Congress of the Czechoslovak Society for Microbiology - Health and Microorganisms, Košice (Slovak Republic), Sept. 5-9, 2001, p. 311 (Po)
- [32]\* Uher M., Hudecová D., Koreňová A., Melník M., Brtko J.: Kojic acid: a natural source for preparation of biological active compounds. In: XLIVth Congress of Science. Katowice (Poland), Sept. 9-13, 2001, S4-P26. (Po)
- [33]\* Urbančíková M., Greifová M., Seemanová Z., Karasová L., Wyatt G.M., Rauch P., Horáková K.: Fluorecence detection of *Listeria monocytogenes* using new antibodies as well as FITC-phalloidin. In: VI<sup>th</sup> International Conference on Agri-Food Antibodies, Prague 2<sup>nd</sup>-5<sup>th</sup> October 2001, Czech Republic, p.104 (Po)
- [34] Urbančíková M., Greifová M., Seemanová Z., Karasová L., Wyatt G.M., Rauch P., Horáková K.: New polyclonal antibodies to *Listeria monocytogenes* give strong reaction by fluorescence microscopy (in Slovak). In: 22nd Congress of the Czechoslovak Society for Microbiology - Health and Microorganisms, Košice (Slovak Republic), Sept. 5-9, 2001, p. 324 (Po)
- [35] Valent A., Kohútová M., Melník M., Švajlenová O., Hudecová D.: Antimikróbna aktivita N-salicylidén-D,L-alaninátových komplexov. Antimicrobial activity of copper complexes of N-salicyl-D,L-alanine (in Slovak). In: 53rd Congress of Chemical Societies. Banská Bystrica (Slovakia), Sept. 3-6, 2000, B-PO29, p. 182-183. (Po)
- [36] Varečka L.: Zvláštnosti homeostázy  $Ca^{2+}$  u vláknitých húb a kvasiniek. Peculiarities of calcium homeostasis in filamentous fungi and yeasts (in Slovak). Drobnicov memoriál, Smolenice (Slovakia), 8.-9.11. 2001, p. 28

## DEPARTMENT OF CERAMICS, GLASS AND CEMENT

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### I. STAFF

#### Associate Professors:

Miroslav Jamnický, PhD, Ján Majling, PhD

#### Assistant Professors:

Jozef Kákoš, PhD, Vladimír Kovár, PhD, Martin T.Palou, PhD, Eva Smrčková, PhD

#### Research Fellows:

Jana Kozánková, Ladislav Pach, PhD, Štefan Svetík

#### PhD Students:

Zuzana Holková, Marian Rebroš, Jaroslav Sedláček, Radovan Tóth

#### Technical Staff:

Ľudmila Illášová, Helena Jablonková, Pavol Krutý, Mária Pelíšková, Iveta Zezulová

#### Emeritus Fellows:

Assoc. Prof. Jozef Laček, PhD, Zdenek Hrabě, PhD

### II. TEACHING AND RESEARCH LABORATORIES

#### A. Teaching Laboratories:

Teaching laboratory I

Teaching laboratory II

#### B. Research Laboratories:

Laboratory of ceramics

Laboratory of glass

Laboratory of inorganic binders

Laboratory of sol/gel

Laboratory of inorganic powders synthesis

Laboratory of thermal analysis

Laboratory of calorimetry

Scanning electron microscopy laboratory

X-ray diffractometer laboratory

### III. TEACHING

#### A. Undergraduate Study

##### 1. Introductory Courses

##### 6th semester (spring)

Materials technology (2-0 h)

Bachelor's thesis (0-4 h)

Majling  
Holková, Jamnický, Kákoš, Kovár,  
Kozánková, Majling, Rebroš, Sedláček,  
Smrčková, Svetík

##### 2. Advanced Courses

##### 7th semester (autumn)

Inorganic chemistry III (2-2 h)

Solid state physics (2-0 h)

Technical mineralogy (1-1 h)

Applied thermodynamics (2-2 h)

Raw materials and mechanical operations (3-0 h)

Specialised laboratory practices I (8 h)

Jamnický  
Lokaj, Smrčková  
Svetík  
Fellner, Pach  
Kovár, Svetík  
Kákoš, Kovár, Kozánková, Palou, Rebroš,  
Smrčková, Svetík

##### 8th semester (spring)

High temperature processes (2-1 h)

Applied heat technique (2-1 h)

Specialised laboratory practices II (8 h)

Kovár  
Kovár, Kákoš  
Holková, Jamnický, Kákoš, Kozánková, Lokaj,  
Manová, Smrčková  
Jamnický, Smrčková

Factory praxis

**9th semester (autumn)**

|                                      |         |   |
|--------------------------------------|---------|---|
| Technology of spec. inorg. materials | (2-0 h) | Majling, Kákoš                                      |
| Inorganic binders technology         | (2-0 h) | Palou   |
| Technology of ceramics               | (2-0 h) | Majling, Smrčková                                   |
| Technology of glass                  | (2-0 h) | Jamnický, Pach                                      |
| Specialised laboratory practices III | (10 h)  | Holková, Jamnický, Majling, Palou, Rebroš, Smrčková |

**10th semester (spring)**

|                            |        |   |
|----------------------------|--------|---|
| Master's thesis laboratory | (30 h) | Galusek, Holková, Jamnický, Kákoš, Kovár, Majling, Pach, Palou, Rebroš, Smrčková, Šimurka |
|----------------------------|--------|---|

**IV. CURRENT RESEARCH PROJECTS****A. Chemical and structural assumption for immobilization of toxic materials by cementing, vitrification and ionic-exchange methods (Ján Majling)**

An appreciable high amount of Cr was accomplished into borosilicate glass by in situ reduction of Cr(VI) by graphite in the first processing step and by subsequent melting and vitrification of the relevant batch.

The toxic Cr(VI) was also immobilized into in situ created ettringite. The laboratory sulfoaluminate cement was used to form ettringite by the hydration process.

The Pb<sup>2+</sup> ions can be incorporated into hydroxyapatite by ionic exchange from solution with respect to the specific surface of hydroxyapatite particles. The substantial exchange can be accomplished only by in situ precipitation of hydroxyapatite from Pb<sup>2+</sup> containing water solutions.

**B. Electrically conductive oxide glasses containing copper cations. Preparation, structure and physical properties (Miroslav Jamnický)**

The possibility to achieve the high ionic conductivity in a new Cu<sup>+</sup> glass system was studied. The main scientific results were obtained as follows:

1. Determination of the optimum procedures for the preparation of electrically conductive oxide glasses containing copper cations in the systems of the general composition CuI – CuBr – Cu<sub>2</sub>O – M<sub>m</sub>O<sub>n</sub> (where M = Mo and W; m = 1 and n = 3).
2. Determination of the arrangement of main structural units in these glasses and characterization of their thermal and electrical properties.
3. Determination of new relationships among the composition, the structure and the electrical conductivity of phosphate, phosphate – molybdate and phosphate – tungstate glasses containing copper ions.

**C. Design microstructure and properties of sol-gel materials by means of seeding and polymer additives (Ladislav Pach)**

The research in the field of sol-gel process synthesis of materials is oriented in the latest time to explanation of  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> crystallisation in boehmite derived alumina gels seeded with Fe(NO<sub>3</sub>)<sub>3</sub>. Our new results, published in three papers, proved, that seeding effect Fe(NO<sub>3</sub>)<sub>3</sub> (system AlOOH - Fe(NO<sub>3</sub>)<sub>3</sub>) is qualitatively different of seeding effect of  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> or  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> crystals in the same boehmite gels. Mechanisms is not crystallographic as in the case of  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> or  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> crystals, but it is a solution effect of dispersed Fe<sup>3+</sup> ions on crystallisation of corundum phase. Ferric oxide originating from Fe(NO<sub>3</sub>)<sub>3</sub> enters into  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> structure resulting in solid solution of  $\gamma$ -(Al, Fe)<sub>2</sub>O<sub>3</sub> and the subsequent process ( $\gamma$ -(Al, Fe)<sub>2</sub>O<sub>3</sub> →  $\alpha$ -(Al, Fe)<sub>2</sub>O<sub>3</sub>) are influenced by Fe<sup>3+</sup> ions, because pure  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> phase is not present. Obtained results enabled us to prepare transparent alumina ceramics at relatively low temperatures about 1300°C

**V. COOPERATION****A. Cooperation in Slovakia:**

Faculty of Electrical Engineering and Information Technology, Slovak University of Technology, Bratislava  
 Faculty of Mechanical Engineering, Slovak University of Technology, Trnava  
 Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava  
 Research Institute of Building Materials, Slovak Academy of Sciences, Bratislava  
 Research Institute of Refractory Materials, Bratislava  
 Cementáreň Turňa, a.s., Turňa nad Bodvou (Cement producer)  
 Považská cementáreň, a.s., Ladce (Cement producer)  
 Hirocem, a.s., Rohožník (Cement producer)  
 Eurodom, s.r.o., Lučenec (Constructional system)  
 Novoker, a.s., Lučenec (Wall tiles producer)  
 CERAM Čáb, a.s., Nové Sady (Electroceramics producer)  
 TS, a.s., Bratislava (Technical glass work)  
 SMZ, a.s., závod Jelšava (Magnesite clinker plant)  
 Izomat, a.s., Nová Baňa (Mineral fibre insulation materials producer)  
 Slovenské elektrárne, Výskumný ústav jadrových elektrární Trnava a.s. (Research institute of electric power stations)

**B. International Cooperation:**

Intercollege Materials Research Laboratory, The Pennsylvania State University, University Park, PA, USA  
 - Synthesis of Inorganic Materials  
 Department of Engineering Materials, The University of Sheffield, U. K.

- Novel Low Energy Cements Based on Belite

### C. Membership in Domestic Organisations and Societies:

Slovak Silicate Society, Bratislava  
 Union of Glass Industry, Bratislava  
 Slovak Glass Society, Lednické Rovne  
 Crystallographic Society, Bratislava  
 Association of Science Technical Societies, Bratislava

### D. Membership in International Organisations and Societies:

Silicate Society, Prague, Czech Republic (Z. Hrabě)  
 American Ceramic Society, USA (L. Pach)  
 The International Society for the Environmental and Technical Implications of Construction with Alternative Materials (ISCOWA),  
 Nederland (J. Majling)  
 Institute of Materials, U.K. (J. Majling)

### G. Visitors from Abroad:

|                             |   |
|-----------------------------|---|
| N. Lyschkow                 | Hamamatsu, Chicago, IL, USA, February 2001 (1 day)                      |
| Prof. Dr. H. Altenburg      | Fachhochschule Münster, Steinfurt, Germany, November 2001 (3 days)      |
| Dipl. Ing. I. Eusch         | Österreichische Heraklith GmbH, Fürnitz, Austria, November 2001 (1 day) |
| Doc. Ing. J. Havlica, DrSc. | FCH VUT, Brno, Czech Republic, December 2001 (2 days)                   |

### H. Visits of Staff Members and PhD Students to Foreign Institutions:

|                        |  |
|------------------------|--|
| M. Rebroš, J. Sedláček | seminar, VŠChT Praha, Czech Republic, February 7-8   |
| P. Krutý               | sample measuring, VŠChT Praha, Czech Republic, May 15  |
| J. Majling             | 7 <sup>th</sup> Conference and Exhibition of the European Ceramic Society, Brugge, Belgium, September 8-13 |
| J. Sedláček            | sample measuring, VŠChT Praha, Czech Republic, September 17  |
| M. Palou, E. Smrčková  | 5 <sup>th</sup> conf. Nové stavební hmoty a výroby, VÚSH Brno, Czech Republic, November 22-23              |

## VI. THESES AND DISSERTATIONS

### A. Graduate Theses (MS Degree) for state examinations after five years of study (supervisors are written in brackets):

|                          |   |
|--------------------------|---|
| Bodorová P.:             | Influence of organic additives on porosity of inorganic gels (L. Pach)  |
| Dominová L.:             | Determination of pc-clinker mineralogical composition by the chemical phase separation (E. Smrčková)  |
| Goliašová-Surgentová A.: | Study of ionic exchange reactions of hydroxyapatite ((E. Smrčková)  |
| Jurenová M.:             | Kinetic evaluation of optical transparency – temperature dependence (V. Kovár)  |
| Kido L.:                 | Fracture properties of polycrystalline corundum (D. Galusek)  |
| Kozloková M.:            | Preparation of the opal-like ordered glassy structure (J. Kákoš)  |
| Michalková E.:           | Study of the mixed anions effect in Cu <sup>+</sup> ionic conductive glasses (M. Jamnický)  |
| Panáček M.:              | Chemical resistance of household glassware in kitchen washers (P. Šimurka)  |
| Radošovská Z.:           | Study of the chemical compositions of solid solutions in the system C-C <sub>2</sub> S-C <sub>3</sub> A-C <sub>4</sub> AF-C <sub>4</sub> A <sub>3</sub> S <sup>+</sup> (J. Majling)                     |
| Rejman J.:               | Identification and verification of singular points relevant for the mixture of raw meal – fly ash – gypsum (M. Palou)   |
| Szatomáry L.:            | Crystallization kinetics of Al <sub>2</sub> O <sub>3</sub> -Fe <sub>2</sub> O <sub>3</sub> gels (L. Pach)   |
| Škorvanová A.:           | Preparation and characterization of products in the system CaO-Al <sub>2</sub> O <sub>3</sub> -SO <sub>3</sub> (CrO <sub>3</sub> )-H <sub>2</sub> O with respect to immobilization of Cr(VI) (M. Palou) |
| Tóth R.:                 | Biocompatible nanocomposites on the base of hydroxyapatite (J. Majling)   |

### B. Dissertations (PhD):

|          |  |
|----------|--|
| Bača L.: | Crystallization of alpha-Al <sub>2</sub> O <sub>3</sub> from boehmite gels (L. Pach) |
|----------|--|

## VII. PUBLICATIONS

### A. Journals (\*registered in Current Contents)

- [1] Alexy P., Košíková B., Crkoňová G., Kozánková J., Martiš P., Precnerová L.: Vplyv EVA kopolymérov na morfológiu a mechanické vlastnosti zmesí polyetylén – lignín. Influence of EVA copolymers on morphology and mechanical properties of polyethylene-lignine mixtures (in Slovak). Ropa, uhlie a petrochémia 43 (1) 42-45 (2001)
- [2]\* Bača L., Lipka J., Tóth I., Pach L.: Study of crystallization of Al<sub>2</sub>O<sub>3</sub>-Fe<sub>2</sub>O<sub>3</sub> gels by Mössbauer spectroscopy. Ceramics –



- Silikáty 45 (1) 9-14 (2001)
- [3]\* Bača L., Plewa J., Pach L., Opfermann J.: Kinetic analysis crystallization of alpha-Al<sub>2</sub>O<sub>3</sub> by dynamic DTA technique. *J. Thermal Analysis and Calorimetry* 66 ( ) 803-813 (2001)
- [4]\* Kákoš J., Bača L., Veis P., Pach L.: Photoluminescence spectra and crystallization of theta-Al<sub>2</sub>O<sub>3</sub> and alpha-Al<sub>2</sub>O<sub>3</sub> from AlOOH-Fe(NO<sub>3</sub>)<sub>3</sub> gels. *J. Sol-Gel Sci. Technology* 21 ( ) 167-172 (2001)
- [5]\* Majling J., Kremničan V., Pach L., Chocholoušek J.: Thermo-optical investigation in transmitted light. *High Temperature – High Pressure* 33 ( ) 43-50 (2001)
- [6] Volfová P., Chrástová V., Černáková L., Mrenica J., Kozánková J.: Properties of polystyrene/poly(butyl acrylate) core/shell polymers modified with N-methyl acrylamide. *Macromol. Symp.* 170 ( ) 283-290 (2001)

## B. Conferences (\*international conferences)

- [1] Bača L., Holková Z., Pach L., Valko M.: Mechanizmy fázovej transformácie böhmitového gélu na korund. Phase transformation mechanisms of boehmite gel to corundum (in Slovak). In: Zb. IV. seminár Príprava keramických materiálov, Herľany, June 26 – 28, 2001, Ed. HF TU Košice, pp. 95-98 (2001), ISBN 80-7099-660-9
- [2]\* Bača L., Plewa J., Wojcik M., Pach L.: Kinetic study of alpha-Al<sub>2</sub>O<sub>3</sub> crystallization in originally AlOOH/Fe(NO<sub>3</sub>)<sub>3</sub> gels. In: Abstracts, 8th Conf. on Calorimetry and Thermal Analysis, Sept. 3-8, 2000, Zakopane (Poland), Ed. AGH Krakow, pp. 235-236 (2000)
- [3]\* Bury P., Jamnický I., Jamnický M.: Acoustic investigation of ion conductive glasses. In: Book of Abstr., 17<sup>th</sup> Int. Congress on Acoustics, Rome (Ital.), Sept. 2-7, 2001, Ed. AIA Roma, p. 121 (2001)
- [4]\* Hockicko P., Bury P., Jamnický I., Jamnický M.: Akustické vlastnosti iónovo vodivých skiel. Acoustic properties of ionic conductive glasses (in Slovak). In: Proc. 6<sup>th</sup> Int. Colloquium Acoustics ICA'01, Zvolen – B. Štiavica, Sept. 19-21, 2001, Ed. TU Zvolen, pp. 17-19 (2001), ISBN 80-228-1048-7
- [5] Holková Z., Pach L.: Nosiče keramických membrán. Ceramic membranes supports (in Slovak). In: Zb. IV. seminár Príprava keramických materiálov, Herľany, June 26 – 28, 2001, Ed. HF TU Košice, pp. 69-72 (2001), ISBN 80-7099-660-9
- [6]\* Holková Z., Pach L.: Príprava keramických membrán. Ceramic membranes preparation (in Slovak). In: Zb. predn. 7. medzinár. konf. Technológia 2001, Bratislava, Sept. 11 – 12, 2001, Ed. STU Bratislava, pp. 57-60 (2001), ISBN 80-227-1567-0
- [7]\* Holková Z., Pach L., Bača L.: Influence of Fe(NO<sub>3</sub>)<sub>3</sub> addition on the porosity of boehmite-derived Al<sub>2</sub>O<sub>3</sub> ceramics. In: Book of abstracts, 6<sup>th</sup> int. conf. on Theoretical and experimental problems of materials engineering, Sept. 5-7, 2001, Ed. Matador Púchov, p. 69 (2001), ISBN 80-968099-5-4
- [8]\* Jamnický I., Bury P., Jamnický M.: Electrical properties of ion conducting glasses. In: Proc. 4<sup>th</sup> Int. Sci. Conf. ELEKTRO 2001, Žilina, May 22-23, 2001, Ed. EF ŽU Žilina, pp. 68-71 (2001), ISBN 80-7100-838-9
- [9]\* Jamnický I., Bury P., Jamnický M., Hockicko P.: Correlation between electrical and acoustical properties of ion conductive glasses. In: Proc. 7<sup>th</sup> Int. Workshop on Applied Physics of Condensed Matter APCOM 2001, Lipt. Mikuláš, Sept. 17-19, 2001, Ed. HONORS Lipt. Mikuláš, pp. 89-92 (2001), ISBN 80-8040-160-8
- [10] Majling J., Kremničan V., Svetík Š., Pach L.: Optická priepustnosť mulitových gélov pri ich ohreve. Optical transmittance of mullite gels at their heat treatment (in Slovak). In: Zb. IV. seminár Príprava keramických materiálov, Herľany, June 26 – 28, 2001, Ed. HF TU Košice, pp. 99-102 (2001), ISBN 80-7099-660-9
- [11]\* Palou M., Majling J.: Application of conduction calorimeter in the study of hydration kinetics of C<sub>2</sub>S-C<sub>4</sub>A<sub>3</sub>S'-CS' system relevant to sulfoaluminat belite cement. In: Sb. prisp. Mezinárodní slovenský a český kalorimetrický seminár 2001, Pribylina, May 28 – June 1, 2001, Ed. B. Taraba, Ostravská univerzita, pp. 103-106 (2001), ISBN 80-7042-803-1
- [12]\* Palou M. T., Smrčková E., Majling J., Pagáčová J.: Vlastnosti cementov s vápencovou prísadou. Properties of cements containing limestone additives (in Slovak). In: Zb. predn. V. konf. Nové stavební hmoty a výroby, Nov. 22-23, 2001, VÚSH Brno, pp. 50-54 (2001)
- [13] Palou M. T., Škorvanová A., Majling J., Smrčková E.: Príprava a charakterizácia produktov v systéme CaO-Al<sub>2</sub>O<sub>3</sub>-SO<sub>3</sub>(CrO<sub>3</sub>)-H<sub>2</sub>O z hľadiska imobilizácie Cr(VI). Preparation and characterization of products in CaO-Al<sub>2</sub>O<sub>3</sub>-SO<sub>3</sub>(CrO<sub>3</sub>)-H<sub>2</sub>O system with respect to immobilization of Cr(VI) (in Slovak). In: Zb. konf. O ochrane životného prostredia vo výrobe nekovových minerálnych produktov a iných priemyselných odvetviach OŽP 2001, Oct. 3-5, 2001, Stará Lesná, ZVVC SR, pp. Q1 – Q11 (2001)
- [14] Petrušková V., Vrabel P., Šimurka P., Maryška M., Rebroš M.: Proces zvetrávania úžitkového skla pri skladovaní. Weathering of household glassware at storing (in Slovak). In: Zb. IV. seminár Príprava keramických materiálov, Herľany, June 26 – 28, 2001, Ed. HF TU Košice, pp. 121-125 (2001), ISBN 80-7099-660-9
- [15] Rebroš M., Petrušková V., Pach L., Šimurka P.: Pôsobenie umývačiek riadu na povrch úžitkového skla. Influence of dish washers on household glassware surface (in Slovak). In: Zb. IV. seminár Príprava keramických materiálov, Herľany, June 26 – 28, 2001, Ed. HF TU Košice, pp. 126-130 (2001), ISBN 80-7099-660-9
- [16] Sedláček J., Jamnický M.: Štúdium zmien mikroštruktúry a zloženia AZS žiaruvzdorných materiálov pri tepelnom zaťažení. Thermal load influence on microstructure and composition of AZS refractory materials (in Slovak). In: Zb. IV. seminár Príprava keramických materiálov, Herľany, June 26 – 28, 2001, Ed. HF TU Košice, pp. 48-52 (2001), ISBN 80-7099-660-9
- [17] Smrčková E., Majling J., Palou M. T.: Imobilizácia toxických odpadov do silikátových matric. Príprava a charakterizácia produktov v systéme CaO-Al<sub>2</sub>O<sub>3</sub>-SO<sub>3</sub>(CrO<sub>3</sub>)-H<sub>2</sub>O z hľadiska imobilizácie Cr(VI). Immobilization of toxic wastes into silicate matrices. Preparation and characterization of products in CaO-Al<sub>2</sub>O<sub>3</sub>-SO<sub>3</sub>(CrO<sub>3</sub>)-H<sub>2</sub>O system with respect to immobilization of Cr(VI) (in Slovak). In: Zb. konf. O ochrane životného prostredia vo výrobe nekovových minerálnych produktov a iných priemyselných odvetviach OŽP 2001, Oct. 3-5, 2001, Stará Lesná, ZVVC SR, pp. Y1 – Y4 (2001)
- [18]\* Smrčková E., Pach L.: Biodegradovateľnosť minerálnych vlákien. Biodegradability of mineral fibres (in Slovak). In: Zb. predn. V. konf. Nové stavební hmoty a výroby, Nov. 22-23, 2001, Ed. VÚSH Brno, pp. 110-113 (2001)
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### C. Books and textbooks

- [1] Collective authors (among them also Majling J., Kovár V., Laček J., Znášik P.): Encyklopaedia Beliana, Slovenská všeobecná encyklopédia v dvanástich zväzkoch. Druhý zväzok Bell-Czy. Encyklopaedia Beliana, Slovak encyclopedia in twelve volumes. Second volume Bell-Czy (in Slovak). EU SAV Bratislava, 2001.
- [2] Koman M., Jamnický M., Majling J.: Anorganické materiály. Inorganic materials (in Slovak). Ed. STU Bratislava, 2001, 165 pp.
- [3] Šimon P., Svetík Š., Smrčková E., Palou M. T.: 1. letná škola termickej analýzy a kalorimetrie, študijné materiály. The first summer school of thermal analysis and calorimetry, textbooks (in Slovak). Ed. FCHPT STU Bratislava, 2001, 62 pp.

## DEPARTMENT OF CHEMICAL AND BIOCHEMICAL ENGINEERING

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### I. STAFF

#### Full Professors:

Vladimír Báleš, PhD, DSc

#### Associate Professors:

Daniel Bobok, PhD, Ján Dojčanský, PhD, Ľudovít Jelemenský, PhD, Jaroslav Longauer, PhD, Jozef Markoš, PhD, Otto Mierka, PhD, Milan Polakovič, PhD, Vladimír Štefuca, PhD

#### Assistant Professors:

Ačai Pavel, PhD, Bafrnec Milan, PhD, Bafrncová Soňa, PhD, Fecková Viera, PhD, Graczová Elena, PhD, Havalda Ivan, PhD, Stopka Ján, PhD, Šefčík Jaroslav, PhD, Šefčíková Milica, PhD, Sokolovská Ivana, PhD, Timár Pavel, PhD, Vajda Milan, PhD

#### Research Fellows:

Antošová Monika, PhD, Besedová Eva, PhD, Godó Štefan, PhD, Hroncová Viera, PhD, Illeová Viera, PhD, Juma Mohammad, PhD, Marták Ján, PhD, Remiarová Bibiana, PhD, Sabolová Erika, PhD, Schlosser Štefan, PhD, Steltenpohl Pavol, PhD, Šoós Miroslav, PhD, Žajdlík Róbert

#### PhD students:

Blažej Michal, Dolgoš Ondrej, Grznárová Gabriela, Kertesz Robert, Klein Jaroslav, Madlová Alexandra, Molnár Attila

#### Technical Staff:

Dobrovodská Mária, Drahošová Anna, Gering Tomáš, Herzán Ľubomír, Hinca Miloš, Chocholová Mária, Luknár Karol, Marenčíková Miroslava, Ördögová Marta, Rizman Viliam

## TEACHING AND RESEARCH LABORATORIES

### A. Teaching Laboratories

Laboratory of Chemical Engineering  
Laboratory of Unit Operations  
Laboratory of Reaction Engineering  
Laboratory of Membrane Processes  
Laboratory of Chemical Engineering Thermodynamics

### B. Research Laboratories

Laboratory of Chemical Reaction Kinetics and Reaction Engineering  
Laboratory of Heat Transfer  
Laboratory of Hydrodynamics and LDA  
Laboratory of Fluid - Particle Dynamics  
Laboratory of Membrane Processes and Membrane Reactors  
Laboratory of Adsorption  
Laboratory of Bioreaction Engineering  
Laboratory of Enzyme Engineering  
Laboratory of Phase Equilibria

## III. TEACHING

### A. Undergraduate Study (Bachelor of Chemical Technology)

#### 1. Introductory Courses

##### 1<sup>st</sup> semester

|  |       |   |
|--|-------|---|
| Material Balances of Technological Processes | (2 h) | M.Šefčíková, P.Ačai, S.Bafrncová, E.Besedová, O.Dolgoš, V.Ileová, M.Kiša, F.Malík, B.Remiarová, P.Steltenpohl, M.Polakovič, J.Šefčík, Š.Sclosser, V.Štefuca, P.Timár, M.Vajda |
|--|-------|---|

##### 5<sup>th</sup> semester

|                        |       |  |
|------------------------|-------|--|
| Chemical Engineering I |       |  |
| Lectures               | (2 h) | V. Báleš, Ľ. Jelemenský  |
| Exercises              | (3 h) | P. Ačai, M. Antošová, S. Bafrncová, D. Bobok, E. Graczová, I. Havalda, O. Mierka, J. Stopka, J. Šefčík, M. Šefčíková, P. Timár, M. Vajda |

|   |         |  |
|---|---------|--|
| Chemical Engineering Laboratory I         | (1 h)   | P.Ačai, M.Antošová, S.Bafrncová, D.Bobok, E.Graczová, G.Grznárová, I.Havalda, M.Juma, R.Kertesz, O.Mierka, J.Longauer, J.Šefčík, M.Šefčíková, P.Timár, M.Vajda                                       |
| <b>6<sup>th</sup> semester</b>            |         |  |
| Chemical Engineering II                   |         |  |
| Lectures                                  | (2 h)   | J.Dojčanský, V.Štefuca, M.Polakovič,   |
| Exercises                                 | (3 h)   | P.Ačai, S.Bafrncová, F.Besedová, D.Bobok, J.Dojčanský, E.Graczová, I.Havalda, O.Mierka, J.Stopka, V.Štefuca, Š.Schlosser, J.Šefčík   |
| Chemical Engineering Laboratory II.       | (3 h)   | P.Timár, P.Ačai, M.Antošová, M.Bafrnec, M.Blažej, E.Graczová, G.Grznárová, I.Havalda, V.Ileová, R.Kertesz, J.Longauer, M.Juma, B.Remiarová, E.Sabolová, P.Steltenpohl, J.Stopka, J.Šefčík, R.Žajdlík |
| Engineering Thermodynamics                |         |  |
| Lectures                                  | (2 h)   | M.Šefčíková, P.Timár   |
| Exercises                                 | (2 h)   | M.Šefčíková, P.Timár, O.Mierka   |
| Technological Projects                    | (4 h)   | M.Bafrnec, J. L.Jelemenský, O.Mierka, A.Molnár, M.Polakovič, Š.Schlosser, M.Polakovič, P.Timár, M.Vajda  |
| Equipment of Chemical and Food Technology | (2-2 h) | J.Longauer   |

**B. Graduate Study (Master of Chemical Technology)**

## 1. Advanced Courses

**7<sup>th</sup> semester**

|  |         |                               |
|--|---------|-------------------------------|
| Chemical engineering Thermodynamics          |         |                               |
| Lectures                                     | (2 h)   | E.Graczová                    |
| Exercises                                    | (2 h)   | E.Graczová,                   |
| Diffusional Separation Processes             | (2-2 h) | J.Dojčanský                   |
| Hydrodynamics and Heat Transfer              |         |                               |
| Lectures                                     | (2 h)   | J.Stopka                      |
| Exercises                                    | (2 h)   | I.Havalda                     |
| Laboratory                                   | (1 h)   | J.Stopka                      |
| Mass Transfer Theorie                        | (2-1 h) | D.Bobok                       |
| Computer Chemical Engineering Calculations   | (3 h)   | M.Juma, A.Molnár, S.Bafrncová |
| Mathematical Methods in Chemical engineering | (4 h)   | I.Havalda                     |

## Safety engineering

|  |          |                               |
|--|----------|-------------------------------|
| Chemical engineering Thermodynamics          |          |                               |
| Lectures                                     | (2 h)    | E.Graczová                    |
| Exercises                                    | (2 h)    | P. Steltenpohl                |
| Hydrodynamics and Heat Transfer              |          |                               |
| Lectures                                     | (3 h)    | J.Stopka                      |
| Exercises                                    | (2 h)    | I. Havalda                    |
| Laboratory                                   | (1 h)    | J.Stopka                      |
| Mass Transfer Theorie                        | (2-1 h)  | D.Bobok                       |
| Fire Engineering                             | (2 -2 h) | K.Balogh                      |
| Computer Chemical Engineering Calculations   | (3 h)    | M.Juma, A.Molnár, S.Bafrncová |
| Mathematical Methods in Chemical Engineering | (4 h)    | I.Havalda                     |

**8<sup>th</sup> semester**

|  |         |  |
|--|---------|--|
| Chemical Engineering                                 |         |  |
| Chemical Reaction Engineering I                      |         |  |
| Lectures   | (2 h)   | J. Markoš  |
| Exercises  | (2 h)   | M. Vajda   |
| Laboratory of Chemical Reaction Engineering          | (2 h)   | J.Markoš   |
| Safety Engineering                                   | (2-2 h) | L.Jelemenský   |
| Bioprocess Engineering I                             |         |  |
| Lectures   | (2 h)   | V.Báleš  |
| Exercises  | (1 h)   | M.Polakovič  |
| Selected Unit Operation                              | (2 h)   | D.Bobok, Š.Schlosser   |
| Project of Equipment of Chemical and Food Technology | (3 h)   | M.Bafrnec, J.Dojčanský, J.Longauer, M.Vajda                                      |
| Advanced Laboratory of Chemical Engineering I        | (3 h)   | J.Šefčík, D.Bobok, E.Graczová, M.Juma, J.Markoš, O.Mierka, B.Remiarová J.Stopka, |

V.Štefuca, Š.Schlosser, P.Timár

## Safety engineering

## Chemical Reaction Engineering I

|  |         |                     |
|--|---------|---------------------|
| Lectures   | (2 h)   | J. Markoš           |
| Exercises  | (2 h)   | M. Vajda            |
| Safety Engineering                                   | (2-2 h) | L.Jelemenský        |
| Explosion Prevention                                 | (2-2 h) | D.Skarba            |
| Process Systems Engineering                          | (2 h)   | P.Rajniak           |
| Laboratory of Process Systems Engineering            | (2 h)   | M.Šoós              |
| Project of Equipment of Chemical and Food Technology | (3 h)   | M.Vajda, J.Longauer |

**9th semester**

|  |         |  |
|--|---------|--|
| Chemical Engineering                           |         |  |
| Chemical Reaction Engineering II               | (2-1 h) | J.Markoš   |
| Process Systems Engineering                    | (1-2 h) | P.Rajniak  |
| Bioprocess Engineering II                      | (1-1 h) | V.Báleš  |
| Design Projekt                                 | (1-1 h) | O.Mierka   |
| Solid Particles in Technology and Environment  | (2 h)   | P.Timár  |
| Cost Engineering of Industrial Enterprise      | (2 h)   | M.Bafrnec  |
| Advanced Laboratory of Chemical Engineering II | (6 h)   | D.Bobok, O.Dolgoš, E.Graczová,<br>L.Jelemenský, I.Langfelder,<br>J.Markoš, O.Mierka, M.Polakovič, B.Remiarová,<br>J.Stopka, V.Štefuca, P.Timár |

## Safety engineering

|  |         |                                   |
|--|---------|-----------------------------------|
| Safety Engineering II                          | (2-2 h) | L.Jelemenský                      |
| Laboratory of Process Plant Safety             | (3 h)   | L.Jelemenský, .Remiarová,         |
| Laboratory of Safety Engineering               | (3 h)   | L.Jelemenský, J.Markoš, J.Stopka, |
| Electrical Saafety for Chemical Process Plants | (1-1 h) | D.Perniš                          |
| Solid Particles in Technology and Environment  | (2 h)   | P.Timár                           |
| Cost Engineering of Industrial Projects        | (2 h)   | M.Bafrnec                         |

**7th semester**

|                                     |       |            |
|-------------------------------------|-------|------------|
| OrganicTechnology                   |       |            |
| Chemical Engineering Thermodynamics |       |            |
| Lectures                            | (2 h) | E.Graczová |

**8th semester**

|                         |       |             |
|-------------------------|-------|-------------|
| Biochemical Engineering |       |             |
| Lectures                | (2 h) | M.Polakovič |

**9th semester**

|                        |       |              |
|------------------------|-------|--------------|
| Safety Engineering     | (2 h) | Ľ.Jelemenský |
| Biochemical Technology |       |              |

**C. Postgraduate study**

|                                 |            |  |
|---------------------------------|------------|--|
| Chemical Engineering            |            |  |
| 1st year:                       | 3 students |  |
| 2nd year:                       | 3 students |  |
| 3rd year:                       | 1 student  |  |
| Obligatory                      |            |  |
| English                         |            |  |
| Mathematics I.,II.              |            |  |
| Chemical Reactors Engineering   |            |  |
| Theory of Mass Transfer         |            |  |
| Hydrodynamics and Heat Transfer |            |  |
| Optional                        |            |  |
| Engineering Bioreactor          |            |  |
| System Engineering              |            |  |

**IV. CURRENT RESEARCH PROJECT****A. Engineering approaches to the investigation of properties of ligand-enzyme-carrier systems in biocatalysis and bioseparations (Milan Polakovič)**

The project incorporates several different problems related to the heterogeneous liquid-solid systems employed in biotechnology. The main areas covered by the project include the optimization of flow microcalorimetry using mathematical modelling for the analytical applications of the biocatalytic systems under study, investigation of enzyme systems with complex kinetics and characterisation of morphological and diffusional properties of carriers used in biocatalysis and biotransformation. The particular goals include the development of methodologies for the identification of mechanisms of enzyme inactivation using the integration of experimental techniques at the quantitative level; the development of chemical

engineering data for the optimization of the design of the fructooligosaccharide production process and for the improvement of biocatalyst properties; the formation of the kinetic equation of triacylglycerols hydrolysis by yeast lipase and its implementation for the description of fermentation production of lipase; modelling of kinetics of potato starch hydrolysis by glucoamylase; the determination of the degree of instability of casein micelles in relation to the degree of hydrolysis of kappa-casein using an experimental procedure of the separation of unstable aggregated micelles and investigation of kinetics of destabilisation of micelles via mathematical modelling of sequential processes; study of the kinetics of glycoprotein sorption at lectin ligands.

### **B. Immobilized biotechnologies: Implementation of new immobilization methods into microbial and plant fermentations and biotransformations, and their industrial applications (Vladimír Štefuca)**

The aim of the project is a systematic development of immobilized biotechnologies. This can be achieved most probably in case of biotechnological processes where the state of the knowledge or the process optimization has reached maximum level and the further increase of the process effectiveness requires the development of new unconventional ways. This evolution should bring more extensive use of continuous processes. The increase of the processes in biotechnology will accelerate their introduction in the industrial use. The project outputs will be information about biochemistry, bioengineering and process parameters that will be used in practical application of investigated processes. The study is oriented toward implementation of immobilization techniques into following processes:

- i) ethanol production by fermentation of starch hydrolysates,
- ii) primary and secondary wort fermentation,
- iii) butyric acid production by transformation of butanol,
- iv) biotransformation/biodegradation of xenobiotics,
- v) secondary metabolite production by plant fermentation.
- vi) dextrose sirup production by maltodextrin hydrolysis.

### **C. Thermal diffusivities of orthogonal anisotropic materials (Milan Bafrnec)**

Elaboration of a model of heat transfer in orthogonal anisotropic composite materials with a course oriented structure. This model will be used for the proposal of a method for measuring thermal diffusivities of such materials. In addition, this method will enable the measurement of the difference in thermal diffusivities in particular directions.

In this year, a suitable mathematical model describing the nonstationary heat transfer in composite materials with a course fiber structure has been proposed. In the choice of parameters and the model of material structure the feasibility solution of the mathematical model was taken into account. Various samples of such composite materials were prepared and their measurement confirmed that there is a great difference between the thermal diffusivity in the direction perpendicular to the fiber layer and in the direction along the composite material fibers.

Models of industrial processes of tire vulcanisation were derived and solved.

### **D. Mathematical and experimental modelling of coal combustion (Jozef Markoš)**

Mathematical and experimental modelling of coal combustion with the aim of its maximal energetic utilization and decreasing of sulphur dioxide emissions.

### **E. Modelling of mass-transfer through membranes and immobilized interfaces directed to formation and modelling of hybrid systems with biochemical or chemical reactions and membrane separation (Štefan Schlosser)**

The possibility of permeate flux enhancement based on the surface modification of a ceramic membrane was investigated in crossflow microfiltration of pure beer yeast suspensions. The stamped membrane had a helical reversed thread to increase turbulence in the feed flow. A stamped membrane has several advantages comparing with a smooth one: flux, as well as limiting flux are higher at the same velocity of the feed, power consumption per unit volume of permeate is lower for the stamped membrane and increases with increasing crossflow velocity of the feed. Modelling of the flux decline indicates different mechanisms of fouling for smooth and stamped membranes.

The mechanism of transport of Ag, phenylalanine (Phe) and other acids through liquid membranes has been studied in a two compartment cell. As carriers for Ag octylphenylmethanesulfide (MF18, novel carrier) and triisobutyl-phosphinesulfide (Cyanex 471X) were used. The advantage of the carrier MF18 is better kinetics of stripping resulting in the same rate of transport or higher in comparison with Cyanex 471X, despite the much lower distribution coefficient of Ag with MF18. The dependence of the transport rate of Phe vs. carrier (DEHPA) concentration goes through a maximum indicating probably aggregation in the membrane phase at higher concentrations of carrier and/or complex. In all systems studied it has been found that the initial flux of permeant through extraction interface is higher than the maximum flux through the strip interface. In some systems this fact leads to a conclusion about the decisive role of kinetics of the processes on stripping interface for the overall transfer rate.

Equilibrium data for butyric acid and dimethylcyclopropanecarboxylic acid with tri-n-octylamine as an extractant have been completed and modelled. These data were interpreted by a chemical reaction mechanism, a related model was tested and the equilibrium constants were estimated. New equilibrium data have been estimated for Phe, silver and HCA.

## **V. COOPERATION**

### **A. Cooperation in Slovakia**

Institute of Chemistry, Slovak Academy of Sciences, Bratislava  
 Institute of Experimental Physics, Slovak Academy of Sciences, Košice  
 Slovak Agricultural University, Nitra  
 LikoSpol, Bratislava  
 Fermas, Slovenská Ľupča  
 SKY Life, s.r.o., Malacky  
 KINEX, a. s.  
 SCP, a.s. Ružomberok

PETROCHEMA, a. s. Dubová  
 RHODIA Industrial Yarns Slovakia, a. s. Humenné  
 Chemical Enterprise Nováky  
 Lhodol, lim. Rajec  
 Combin, lim. Tisovec  
 Research Institute for Milk Products, Žilina  
 Slovakofarma, a.s. Hlohovec

## B. International Cooperation:

CIBA, Swiss  
 - synthesis of IRGANOX L67  
 Wroclaw Institute of Technology, Wroclaw, Poland  
 - starch hydrolysis and starch enzyme inactivation  
 Laboratoire Environnement et Minéralurgie, UMR INPL et CNRS N° 7569, Nancy, France  
 - organic pollutants removal from drinking water by activated coal adsorption  
 University of Lund, Lund, Sweden  
 - flow microcalorimetry  
 Oakland University, Rochester, USA  
 - amperometric sensors for the determination of NO  
 - monitoring of new anticancer drugs by HPLC  
 University of Perugia, Perugia, Italy  
 - study of cyanocomplexes of Cr  
 - development of thermometric sensors for investigation of enzyme properties  
 Institute für Technische Chemie der Universität Hannover, Hannover, Germany  
 - immobilized enzymes applications  
 Bundesforschungsanstalt f. Landwirtschaft (FAL), Braunschweig, Germany  
 - immobilized enzymes applications  
 Consejo superior de investigaciones científicas, Madrid, Spain  
 - investigation of immobilized enzyme stability and inactivation  
 Academy of Sciences of Czech Republic, Prague, Czech Republic  
 - study of properties of immobilized lipases  
 Lab. Membrane Mater. Proc. ENSCM, Montpellier, France  
 - joint project INCO Copernicus  
 ICMAB, Barcelona, Spain  
 - joint project INCO Copernicus  
 Amino GmbH, Hannover, Germany  
 - joint project INCO Copernicus  
 BCS Engineering, Brno Czech Republic  
 - joint project INCO Copernicus  
 Technical University of Bucharest, Romania  
 - joint project INCO Copernicus  
 Res. Centre Macromolecular Materials and Membranes, Bucharest, Romania  
 - joint project INCO Copernicus  
 Technical University of Warsaw, Poland  
 - joint project INCO Copernicus  
 Aston University, Birmingham, UK  
 - joint project INCO Copernicus  
 Universidade do Minho, Braga, Portugal  
 - joint project INCO Copernicus  
 University College London, United Kingdom  
 - Grant British Council/STU Bratislava  
 Acetec, Vienna, Austria  
 - EUREKA  
 Scheidl Umweltanalytic, Vienna, Austria  
 - EUREKA  
 VUOS Pardubice, Czech Republic  
 - research cooperation in the EURECA programme

## C. Membership in Domestic Organisations and Societies:

Slovak Society of Chemical Engineering (chairman: V. Bálež, member of the general committee: Š. Schlosser)  
 Slovak Society of Biotechnology (chairman: V. Bálež)

## D. Membership in International Organisations and Societies:

European Membrane Society, Toulouse, France (Š. Schlosser, member of the Council)  
 European Federation of Chemical Engineering (Š. Schlosser, Slovak delegate of the Working Party for Membranes)  
 European Federation of Chemical Engineering (V. Bálež, member of the Executive Board)  
 European Federation for Biotechnology (M. Polakovič, member of the Working Party for Applied Biocatalysis)  
 European Federation for Biotechnology (V. Bálež, member of the Working Party for Bioreactor Performance and Slovak delegate in the General Assembly)  
 American Chemical Society (V. Bálež, member)

**E. International Scientific Programs:****1. COPERNICUS**

a/ Inco-Copernicus ERBIC15 CT98 0809." Novel techniques for implementation of immobilized biocatalysts in industrial processes"

Scientific partner at STU: Dr. Vladimír Štefuca

Coordinator: Dr. Bengt Danielsson (Lund University, Sweden)

Other partner institutions: FAL Braunschweig (D), Technical University of Hannover (D), Amino GmbH, Hannover (D), CSIC, Madrid (E), SAS, Bratislava (SK), AS CR, Prague (CR), BCS Engineering, Brno (CR).

The project started: 1.9.1998

Duration of the project: 3 years

A research project of 7 partners from EU countries, 2 from the Czech Republic, and 2 from Bratislava. It is a Concerted Action project aimed at creating links among partners, research coordination and preparing possible future actions. No money for the research support is available if not the financial support provided by the EU for this project. The main objective of the project is to facilitate the implementation of new materials and techniques into industrial biocatalytic processes. The project involves interdisciplinary trans-national teams to integrate expertise on immobilized biocatalysts. Expertise of partners covers, in particular, the development of the carriers for immobilization, immobilization techniques, methods of characterisation of immobilized biocatalysts, novel approaches for biotransformations, development of bioreactors with immobilized biocatalysts, process monitoring and control, and scaling up processes.

b/ Inco-Copernicus IC15-CT98-0904: "Modelling and design of multiphase bubble bed reactors for advanced food industries"

Responsible at STU: Jozef Markoš

Coordination institution: Aston University, Birmingham, UK

Other partner institutions: Universidade do Minho, Braga, P, Institute of Chemical Processes, Czech Academy of Sciences, Prague CZ.

Duration of the project: November 1998 - October 2001

**2. Grant STU/British Council: "Process simulation for environmental and safety assessment"**

Responsible at STU: Ľudovít Jelemenský

Coordination institution: University College London.

Duration of the project: 1999 - 2001

**3. EUREKA**

EUREKA EU 1574: "Lowering Occurrence and Diminishing Effluents/ Pollution at Source - Treatment and Recovery" (acronym: LODE (P) STAR)

Responsible at STU: Štefan Schlosser

Coordinated by VÚOS, Pardubice, Ing. Josef Kotlán

Other partners: Acetec, Vienna (A), Scheidl Umweltanalytic, Vienna (A).

Duration of the project: 1998-2000.

**4. INCO Copernicus Programme**

IC15-CT98-0147: "Recycling heavy metal ions and organics of biological interest by innovative separation membranes"

Responsible at: STU Štefan Schlosser

Coordinated by Lab. Membrane Mater. Proc. ENSCM, Montpellier (F)

Other partners Technical University of Bucharest (RO), Res. Centre Macromol. Materials Membranes, Bucharest (RO), Warsaw University of Technology (PL), Inst. of Material Science of Barcelona (E).

Duration of the project: January 1999 – 2001

**F Visitors from Abroad:**

Dr. J. Bryjak

Wroclaw Institute of Technology, P, August 2000, 5 days

Dr. B. Danielsson

Lund University, S, October 2000, 3 days

Prof. David Bogle

UCL London, UK, January 2000 (4 days)

Prof. Eric Fraga

UCL London, UK, January 2000 (4 days)

Prof. Jose Luis Rico Cerda

Universidad Michoacana, Morelia, Mexico, July 2000, (2 days)

Ing. Quido Smejkal, PhD

VŠCHT Praha, CZ, November 2000 (2 days)

J. Kotlán, M. Havlík

VÚOS, a.s., Pardubice, CZ, January, May and December 2000 (3 days)

G. and A. Vladislavjevič

Inst. Food Technol. Biochem., Univ. Belgrade, YU, June 2000 (3 days)

J-A. Jonsson, Dept. Analyt. Chem.

Lund Univ., Lund, S, September 2000, (2 days)

P. Uchytíl

Inst. Chem. Proc. ASCR, Praha, CZ, November 2000 (3 days)

**G. Visits of Staff Members and PhD Students to Foreign Institutions:**

D. Bobok

Technische Universität, Munich, Germany, January 2000 (3 days)

M. Polakovič

2nd International Conference on Protein Stabilisation/Biomolecule Stabilisation, Lisbon, Portugal, April 9-12, 2000.

V. Štefuca

2nd International Conference on Protein Stabilisation/Biomolecule Stabilisation, Lisbon, Portugal, April 9-12, 2000.

M. Polakovič

ISCRE 16 – 16th International Symposium on Chemical Reaction Engineering, Cracow, Poland, September 10-13, 2000.

Ľ. Jelemenský

Ljubljana, Slovenia, September 2000, (3 days)

D. Bobok

14<sup>th</sup> International Congress CHISA, Prague, CZ, August 2000, (4



|                           |   |
|---------------------------|---|
| L. Jelemenský             | days)<br>14 <sup>th</sup> International Congress CHISA, Prague, CZ, August 2000, (4 days)     |
| J. Markoš                 | 14 <sup>th</sup> International Congress CHISA, Prague, CZ, August 2000, (4 days)              |
| B. Remiarová              | 14 <sup>th</sup> International Congress CHISA, Prague, CZ, August 2000, (4 days)              |
| M. Šoóš                   | 14 <sup>th</sup> International Congress CHISA, Prague, CZ, August 2000, (4 days)              |
| O. Dolgoš                 | 14 <sup>th</sup> International Congress CHISA, Prague, CZ, August 2000, (4 days)              |
| J. Klein                  | 14 <sup>th</sup> International Congress CHISA, Prague, CZ, August 2000, (4 days)              |
| Š. Schlosser, E. Sabolová | 14 <sup>th</sup> International Congress CHISA, Prague, CZ, August 2000, (4 days)              |
| L. Jelemenský             | International Symposium on Chemical Reactor Engineering, Krakow, PL, September 2000, (3 days) |
| J. Markoš                 | International Symposium on Chemical Reactor Engineering, Krakow, PL, September 2000, (3 days) |
| J. Markoš                 | UCL London, UK, October 2000, (1 week)  |
| M. Šoóš                   | UCL London, UK, October 2000, (1 week)  |
| J. Markoš                 | Universidade do Minho, Braga, P, April 2000, (4 days)   |
| J. Markoš                 | ETH Zurich, Zurich, Switzerland, April 2000, (1 day)  |
| Š. Schlosser              | Meeting of the EMS Council at CNRS Paris, January 2000 (4 days)                               |
| Š. Schlosser              | EIDOS, a.s., Zlín, CZ, April 2000, (1 day)  |
| Š. Schlosser              | meeting of the INCO Copernicus project, Bucharest, RO, June 2000 (3 days)                     |
| R. Kertész                | Young Membrains, Aachen, D, June 2000, (4 days)   |
| J. Stopka, Š. Schlosser   | ICIM2000, Montpellier, F, June 2000 1999 (8 days)   |
| Š. Schlosser              | Euromembrane 2000, Maale Hachamisha, Israel, September 2000 (7 days)                          |
| M. Bafrnec                | Conference New Trends in Rubber Industry, Zlín, CZ, November 2000                             |

## VI. THESES AND DISSERTATIONS

### A. Graduate Theses (MS Degree) for state examinations after five years of study (supervisors are written in brackets):

|                   |   |
|-------------------|---|
| Báleš, J.:        | Complex design of a tube heat exchanger considering possible phase transfers in both media (I. Langfelder)                                    |
| Baláž, P.:        | Evaluation of the influence of rheological properties and conditions of the application of a starch solution on final paper drying (P. Timár) |
| Blažej, M.:       | Fermentation in an airlift reactor (J. Markoš)  |
| Bořanský, B.:     | Investigation of structural properties of a single coal particle in the combustion process. (B. Remiarová)                                    |
| Hubinová, M.:     | Safety analysis by the aid of the HYSYS program (M. Šoóš)   |
| Hudecová, M.:     | Kinetics of coal combustion (L. Jelemenský)   |
| Józsa, K.:        | Energy audit at real conditions of a production plant (O. Mierka)   |
| Kertész, R.:      | Pertraction of organic acids from model and fermentation solution in a fiber contactor (Š. Schlosser)   |
| Kováčová, K.:     | Pertraction of metals – mass transfer. (M. Vajda)   |
| Krošlák, M.:      | Fermentation in an airlift reactor (J. Markoš)  |
| Kvinta, F.:       | Safety assessment of the reactive distillation by the aid of the HYSYS program. (L. Jelemenský)   |
| Laurinc, T.:      | Safety analysis of chemical reactors. (J. Markoš)   |
| Mikulová, E.:     | Mass transfer in a fiber contactor. (M. Vajda)  |
| Petergáčová, Z.:  | The influence of model substances on the decrease of flux of permeate in microfiltration through ceramic membranes. (J. Stopka)               |
| Porubská, I.:     | Modelling of chromatographic processes of removal of organic impurities from potable water. (M. Polakovič)                                    |
| Pristyákková, Z.: | Design of a high temperature heat pump operating with a solution LiBr-H <sub>2</sub> O (I. Langfelder)  |
| Pšenák, M.:       | Experimental investigation of diffusion of water in silicagel particles (D. Bobok)  |
| Račko, D.:        | Mathematical modelling of controlled drug release (M. Polakovič)  |
| Sirková, Ž.:      | Removal of heavy metals from waste waters by sorption on microbial biomass (M. Polakovič)   |
| Skokan, S.:       | Spread of pollutants in the air (J. Stopka)   |
| Zavdil, V.:       | Kinetics of coal combustion in the atmosphere of carbon dioxide (L. Jelemenský)   |

Zuber, J.: Possibilities of utilisation of the software CAMEO for the creation and assessment of realistic scenarios of accidents (V. Fecková)

## B. Dissertations (PhD):

Klein, J.: Study of transport processes in airlift reactors with model and fermentation processes  
 Juma, M.: Nonstationary heat transfer and thermal diffusivity of composite materials.

## VII. PUBLICATIONS

### A. Journals (\*registered in Current Contents)

- [1] Bobok D., Besedová E.: Error in the Estimation of Effective Diffusion Coefficients from Sorption Measurement. *Chem. Papers* 54 (6b), 482-488 (2000)
- [2] Bugan, G. S., Dömény, Z., Šmogrovičová, D., Stopka, J., Schlosser, Š.: Aplikácia mikrofiltrácie pri odhorčovaní odpadových pivovarských kvasiniek pre potravinárske účely. *Bulletin potravinárskeho výskumu (Application of microfiltration in debittering of waste beer yeast for foostaff purposes (in Slovak))* 39 203-211 (2000)
- [3] Bugan, G. S., Dömény, Z., Šmogrovičová, D., Švitel, J., Šturdík, E., Stopka, J., Schlosser, Š.: Ceramic membrane cross-flow microfiltration for beer recovery from tank bottoms. *Monatsschrift für Brauwissenschaft* 53, 229-233 (2000)
- [4] Jelemenský L., Markoš J., Žajdlík R., Remiarová B.: Modelling of non-linear behaviour during combustion of single coal particle. *Chem. Papers* 54, (6b) 473-481 (2000)
- [5] Juma M., Bařmec M.: Method of Measuring Thermal Diffusivity of Composites with Thick Fillers and Reinforced Rubbers. *Journal of Reinforced Plastics and Composites* 19, 1024-1031(2000)
- [6] González-Velasco, J.R., López-Fonseca, R., Aranzabal, A., Gutiérrez-Ortiz, J.I., Steltenpohl, P.: Evaluation of H-Y type Zeolites in the Destructive Oxidation of Chlorinated Volatile Organic Compounds. *Appl. Catal. B: Environmental* 24, 233-242 (2000)
- [7] Klein, J., Dolgoš, O., Blažej, M., Markoš, J., Godó, Š.: Application of a magnetic tracer method for the characterisation of hydrodynamics in internal – loop airlift bioreactors. *Chemical Papers* 54, (6b) 456-466 (2000)
- [8] López-Fonseca, R., Aranzabal, A., Steltenpohl, P., Gutiérrez-Ortiz, J.I., González-Velasco, J.R.: Performance of Zeolites and Product Selectivity in the Gas-Phase Oxidation of 1,2-Dichloroethane. *Catal. Today* 62, 367-377 (2000)
- [9] Madlová, A., Antořová, M., Polakovič, M., Báleš, V. Thermal stability of fructosyltransferase from *Aureobasidium pullulans*. *Chemical Papers* 54 (6a), 339-344 (2000)
- [10] Madlová, A., Antořová, M., Baráthová, M., Polakovič, M., Štefuca, V., Báleš, V. Biotransformation of sucrose to fructooligosaccharides: the choice of microorganisms and optimization of process conditions. *Food Biotechnology (Bielecki, S., Tramper, J., Polak, J. eds). Progress in Biotechnology, Vol. 17, Elsevier, Amsterdam, 151-155 (2000)*
- [11] Markoš, J., Jelemenský, L.: Bezpečnostné inžinierstvo na Katedre chemického a biochemického i nžinierstva STU v Bratislave. Safety engineering at the Department of Chemical and Biochemical Engineering of the STU in Bratislava (in Slovak). *Ropa, uhlie, plyn a petrochémia* (42) 17-20 (2000)
- [12] Marták, J., Schlosser, Š.: L/L Equilibria of Dimethylcyclopropanecarboxylic Acid in Water - Solvent Systems with Trioctylamine as an Extractant. *Chem. Papers* 54, 413-422 (2000)
- [13] Mierka O., Timár P.: Criterial Equation of Pressure Losses by Vertical Pneumatic Transport. *Powder Handling and Processing* 4 (2000)
- [14] Sokolovská, I., Polakovič, M., Báleš, V.: Kinetics of olive oil hydrolysis by *Candida cylindracea* lipase. *Food Biotechnology (Bielecki, S., Tramper, J., Polak, J. eds) Progress in Biotechnology, Vol. 17, Elsevier, Amsterdam, 209-214 (2000)*
- [15] Stopka, J., Schlosser, Š., Dömény, Z., Šmogrovičová, D.: Flux Decline in Microfiltration of Beer and Related Solutions of Model Foullants through Ceramic Membranes. *Polish Journal of Environmental Studies* 9, 65-69 (2000)
- [16] Šefčíková M., Šefčík J., Báleš V.: Kinetic parameters of casein protein coagulation. *Chemical Papers* 53, 370-373 (1999)
- [17] Šefčíková M., Šefčík J., Šefčík J., Báleš V.: Kinetics of casein micelle destabilization. *Chemical Papers* 54, 345-350 (2000)
- [18] Šoóš, M., Rajniak, P.: Mathematical and experimental modelling of sorption processes in a fixed bed adsorber. *Chem. Papers* 54, (6b) 489-495 (2000)
- [19] Štefuca, V., Polakovič, M.: The use of enzyme flow microcalorimetry for determination of soluble enzyme activity. *Food Biotechnology (Bielecki, S., Tramper, J., Polak, J. eds) Progress in Biotechnology, Vol. 17, Elsevier, Amsterdam, 353-358 (2000).*
- [20] Štěpánek, F., Kubicek, M., Marek, M., Rajniak, P., Soos, P., Yang, R.T.: On the modelling of PSA cycles with hysteresis-dependent isotherms. *Chemical Engineering Science* 55, 431-440 (2000)
- [21] Vajda, M., Schlosser, Š., Kováčová, K.: Pertraction of Silver through Bulk Liquid Membranes. *Chem. Papers* 54, 423-429 (2000)
- [22] Žajdlík, R., Markoš, J., Jelemenský, L., Remiarová, B.: Single Coal particle Combustion in Different Oxygen Atmosphere. *Chem. Papers* 54, (6b) 467-472 (2000)
- [23] Žajdlík, R., Markoš, J., Remiarová, B., Jelemenský, L.: Mathematical and Experimental Modelling of Coal Combustion (Review). *Petroleum and Coal* 42, 71 - 87 (2000)

### B. Conferences (\*international conferences)

- [1] Ačai, P., Michálková E., Báleš, V.: Mathematical modelling of a packed bed bioreactor with immobilized permeabilized cells of *Trigonopsis variabilis*. In: *Proceedings of the 27th International Conference of the Slovak Society of Chemical Engineering, Tatranské Matliare, Slovakia, May 22.-26. 2000, B5 (CD ROM), 19 pp.*
- [2] Ačai, P., Michálková E., Báleš, V. : Mathematical analysis of the performance of a packed bed bioreactor with immobilized permeabilized cells. In: *Proceedings of the 14th International Congress CHISA, Praha, Czech Republic, August 27.-31. 2000, P5.79 (CD ROM), 18 pp.*
- [3] Bařmcová S., Havalda I., Graczořová E: Calculation of VOC Emission from Industrial Wastewater Treatment. In: *Proceedings*

- of the 27th International Conference of the Slovak Society of Chemical Engineering, Tatranské Matliare, Slovakia, May 22.-26. 2000, B5, p.74
- [4] Bafnec M., Juma M. : Chemical engineering aspects of tyre vulcanisation. In: Proceedings of the Slovak Rubber Conference 2000, Púchov, Slovakia, 23.-24. May 2000
- [5] Bafnec M., Juma M.: Analysis of the Tyre Curing Process in a Press with Diaphragm Heated by Steam and Nitrogen. In: Proceedings of the 27th International Conference of Slovak Society of Chemical Engineering, Tatranské Matliare, Slovakia, May 22.-26. 2000, p. 70
- [6] Bafnec M., Juma M. : Tire Curing Engineering. In: Proceedings New Trends in Rubber Industry 2000, Zlín, Czech Republic , November 7.-8. 2000, p. 137
- [7] Bálež, V. Ačai, P.: Strategy for the application of Immobilized biocatalyst. In: Proceedings of the 14th International Congress of Chemical and Process Engineering. Praha, Czech Republic, August 27.-31. 2000, A5,1(CD ROM), 4 pp.
- [8] Bobok D., Besedová E.: Diffusional Mass Transfer in Porous Solids. In: Proceedings of the 27-th International Conference of the Slovak Society of Chemical Engineering. Tatranské Matliare, Slovakia, May 22.-26. 2000, 14pp. (CD ROM), ISBN 1 80-227-1350-3
- [9] Bobok D., Besedová E.: Error in the Estimation of Effective Diffusion Coefficients from Sorption Measurements. *ibid*, 12pp.
- [10] Bobok D., Bodnár Z., Besedová E.: Diffusion of Water in Particles of Silicagel. In: Book of Abstracts of the 14th International Congress CHISA 2000. Praha, Czech Republic, August 27.-31. 2000, D6.5
- [11] Besedová E., Bobok D.: Evaluation of Isosteric Heats from Adsorption Equilibrium Measurements. In: Proceedings of the 27-th International Conference of the Slovak Society of Chemical Engineering. Tatranské Matliare, Slovakia, May 22.-26. 2000, (CD ROM), ISBN 1 80-227-1350-3, P 213, 6pp.
- [12] Besedová E., Bobok D.: Isosteric Heat as a Part of Adsorption Equilibrium. In: Book of Abstracts of the 14th International Congress CHISA 2000, Praha, Czech Republic, August 27.-31. 2000, P3.140
- [13] Bugan, G.S., Stopka, J., Broussous, L., Schlosser, Š., Larbot, A.: Vplyv tvarovaného povrchu keramickej membrány na tok permeátu. The influence of the stamped surface of a ceramic membrane on the flux of permeate (in Slovak). In: Proceedings of the 27th International Conference of the Slovak Society of Chemical Engineering, full texts on CD ROM, Tatranské Matliare, Slovak Republic, May 22. – 26. 2000, 4 pp.
- [14] Dolgoš, O., Klein, J., Blažej, M., Polák, Š., Annus, J., Markoš, J.: Measurements of circulation velocity in internal-loop airlift bioreactors using a new magnetic – tracer method. In: Proceedings of the 27th International Conference of the Slovak Society of Chemical Engineering, Tatranské Matliare, SK, May 22.– 26. 2000, p. 52
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- [18] Hajdučíková, L., Koniarová, D., Polakovič, M., Rehák, L., Bakoš, D.: The mechanism and kinetics of drug release from biodegradable membranes. In: Proceedings of the 27th International Conference of the Slovak Society of Chemical Engineering, Tatranské Matliare, Slovakia, May 22.-26. 2000, P309 (CD ROM), 5 pp.
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- [20] Illeová, V., Štefuca, V., Polakovič, M.: Investigation of enzyme inactivation by flow calorimetry. In: Conference Application of Biotechnology in Agriculture and Food Production. Nitra, Slovakia, October 3.-5. 2000, S23 (poster)
- [21] Jelemenský, L., Markoš, J., Žajdlík, R., Remiarová, B.: Modelling of non-linear behaviour during combustion of single coal particle. In: Proceedings of the 27th International Conference of the Slovak Society of Chemical Engineering, (CD), Tatranské Matliare, SK, May 22. – 26. 2000
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- [23] Jelemenský, L., Šoóš, M., Markoš, J.: Dynamical simulation of safe control of MTBE reactive distillation. In: Book of Abstracts of the 14th International Congress CHISA. Praha, CZ, August 27. –31. 2000
- [24] Juma M., Bafnec M. : Nonstationary heat transfer in reinforced rubber products. Proceedings of the Slovak Rubber Conference 2000, Púchov, Slovakia, 23.-24. May 2000
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- [29] Klein, J., Bálež, V., Godó, Š.: Comparative study of citric acid fermentation in various types of bioreactors. In: Proceedings of the 3rd European Symposium on Biochemical Engineering Science (ESBES III), Copenhagen, Denmark, September 10.-13. 2000, p.176
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- [36] Mierka O, Timár P.: Cogeneration in Industrial units of Middle Spread. In: Proceedings of the 27-th International Conference of the Slovak Society of Chemical Engineering, Tatranské Matliare, May 2000, p. 177
- [37] Molnár, A.: The run-away phenomena in plug flow reactors. In: Proceedings of the 27th International Conference of the Slovak Society of Chemical Engineering, (CD), Tatranské Matliare, SK, May 22. – 26. 2000, p. 94
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- [44] Sabolová, E., Schlosser, Š.: Pertraction and membrane based solvent extraction of butyric acid in hollow fiber contactors. In: Proceedings of the 14th International Congress CHISA 2000, (CD), Praha, Czech Republic, August 28. –31. 2000, 13 pp.
- [45] Serrano-Sánchez, A.M., Steltenpohl, P., González-Marcos, M.P., González-Velasco, J.R.: Stabilizing Effect of Platinum on Supported Ruthenium/Zirconia Catalysts. In: Book of Abstracts of the 14th International Congress CHISA 2000, Praha, Czech Republic, August 27.-31. 2000, P5.154
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- [47] Schlosser, Š.: Pertraction of organic acids and silver through liquid membranes, invited lecture at the Technical University of Bucharest, Romania. (June 8, 2000)
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- [60] Timár P., Mierka O.: Cogeneration - Modern Solution of Energy Media Production in Industrial Enterprises. In: Proceedings of the 27-th International Conference of the Slovak Society of Chemical Engineering. Tatranské Matliare, Slovak Republic, May 22.-26. 2000, p. 178
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- [62] Vajda, M., Schlosser, Š., Kováčová, K., Teixidor, F.: Pertraction of Silver with Octylphenylsulfide as a Carrier. In: Proceedings of the 14th International Congress CHISA 2000, (CD ROM), Praha, Czech Republic, August 28.-31. 2000, 8 pp.
- [63] Vajda, M., Schlosser, Š. \*, Kováčová, K., Teixidor, F.: Pertraction of silver through bulk liquid membranes. In: Procédés á membrane dans la protection de l'environnement, Bucurest , 2000 RO
- [64] Žajdlík, R., Markoš, J., Jelemenský, L., Remiarová, B., Zavadiľ, V.: Single coal particle combustion in CO<sub>2</sub> atmosphere. In: Proceedings of the 27th International Conference of the Slovak Society of Chemical Engineering, (CD), Tatranské Matliare, SK, May 22. – 26. 2000, p. 18
- [65] Žajdlík, R., Markoš, J., Jelemenský, L., Remiarová, B., Hudecová, M.: Single Coal Particle Combustion in Different Oxygen Atmosphere. In: Proceedings of the 27th International Conference of the Slovak Society of Chemical Engineering, Tatranské Matliare, SK, May 22. – 26. 2000, p. 168
- [66] Žajdlík, R., Jelemenský, L., Remiarová, B., Markoš, J.: Experimental and modelling investigation of single coal particle combustion. In: Book of abstracts ISCRE 16, Krakow, Poland, September 10. – 13. 2000

### C. Books and Textbooks

- [1] Bafrcová S., Šefčíková M., Vajda M.: Chemické inžinierstvo, Tabuľky a grafy. Chemical Engineering. Tables and Graphs (in Slovak). STU Bratislava, 2000, ISBN 80-227-1304-X
- [2] Dojčanský J., Longauer J.: Chemické inžinierstvo II. Chemical Engineering II (in Slovak). Malé centrum 2000, ISBN 80-967064-8-9
- [3] Schlosser, Š.: Membrane Based Processes with Immobilized Interface. In: Integration of Membrane Processes into Bioconversions. Kluwer Academic, p. 55-72 (2000)
- [4] Schlosser, Š.: Pertraction Through Liquid and Polymeric Membranes. In: Integration of Membrane Processes into Bioconversions. Kluwer Academic, p. 73-100 (2000)
- [5] Schlosser, Š.: Membránové procesy. Membrane processes (in Slovak). In: Chemické inžinierstvo II. (Chemical Engineering II (in Slovak)). J. Dojčanský, J. Longauer, Malé centrum, Bratislava, p. 333-374 (2000)

### D. Reports and Invited Lectures

- [1] Bafnec, M. : Course: „Engineering aspects of new rubber technologies“. Barum-Continental, April 27.-28. 2000, Luhačovice, CZ
- [2] Bafnec M, Havalda, i., Langfelder I., Mierka O., Timár P.: Course: „Management in the production of paper“. Course for SCP Ružomberok, January-March, 2000
- [3] Bafnec M.: Engineering of rubber productions. 9th semester 2000/2001 lectures 4h/week, Faculty of Industrial Technologies in Púchov, University of Trenčín
- [4] Bafnec M.: Method for estimation of the vulcanisation degree. Research report for Matador a. s. Púchov, Slovakia
- [5] Bafnec M. Juma M.: Reduction of the energy consumption in the rubber production. Research report for Matador a. s. Púchov, Slovakia
- [6] Bobok D.: Diffusion of Water in Particles of Silicagel. Thermodynamikseminar, TU München, 28.1.2000, pp.11 (invited lecture)
- [7] Hudec I. Alexy P. Bafnec M. Juma M. aet al.: Dynamico-mechanical properties and thermal diffusivity of components used for the production of tires. Research report for Matador a. s. Púchov, Slovakia
- [8] Jelemenský L., Šoóš M., Markoš J.: Chemical-engineering calculations and modification of the rectification column for the mixture DFA, nonene and additives. Research report for CIBA, Swiss (2000)
- [9] Jelemenský, L., Markoš, J.: Safety engineering, lectures within the frame of the education of the staff in SCP, a.s., Ružomberok, November – December, 2000
- [10] Markoš M., Jelemenský L., Šoóš M.: Chemical-engineering calculations of a reactor and absorber for the production of chloroethanol Research report for Novácke Chemické Závody, a.s., Nováky (2000)
- [11] Markoš J., Jelemenský L., Šoóš M.: Kinetics of synthesis of IRGANOX L67. Research report for CIBA, Swiss (2000)
- [12] Markoš J., Jelemenský L., Šoóš M.: Estimation of basic physical properties of porous materials (surface area, mean radius of pores, specific volume of pores distribution of pores according to size, porosity) by the apparatuses SORPTOMATIC 1900 a POROSIMETER 2000 for:  
Lhodol, s.r.o, Rajec,  
Combin, s.r.o., Tisovec,  
SCP a.s. Ružomberok,  
Novácke chemické závody, a.s. Nováky
- [13] Markoš J., Klein J.: Rheological measurement of samples of milk products by VISKOTESTER VT 550. Research report for the Research Milk Institute, Žilina (2000)
- [14] Markoš J.: Chemical substances and environment, invited lecture for the advanced education of managers in SLOVAKOFARMA, a.s., Hlohovec, November 2000
- [15] Markoš, J.: Experimental and mathematical modelling of single coal particle combustion. ETH Zurich, Switzerland, April 2000 (invited lecture)
- [16] Mierka O., Timár P.: Material and energy balance of an evaporator for black liquor after its reconstruction. Research Report for SCP, a.s. Ružomberok
- [17] Mierka O., Timár P, Langfelder I.: Elaboration of an energy audit for the regeneration of caprolactam. Research Report for

- RHODIA Industrial Yarns Slovakia, a. s. Humenné
- [18] Schlosser, Š.: Pertraction of organic acids and silver through liquid membranes, Technical University of Bucharest, Bucharest, RO, June 8, 2000. (invited lecture)
  - [19] Šoóš M.: Applicability of the software HYSYS for safety analysis. University College London, London, UK, October, 2000 (invited lecture)
  - [20] Timár P., Mierka O., Báleš V.: Decrease of energy, and consumption of heat and pressurised air. Research Report for SKY Life, lim., Malacky
  - [21] Timár P., Mierka O., Báleš V. : Decrease of energy in the production of pressurized air. Research report for KINEX, a. s.
  - [22] Timár P., Mierka O., Báleš V.: Analysis of the efficiency of heat consumption in Petrochema Dubová. Research Report for PETROCHEMA, a. s. Dubová
  - [23] Timár P., Mierka O. : Course aimed at special problems of energy in industrial enterprises, for FERMAS s. r. o. Slovenská Lupča (2000)

## DEPARTMENT OF CHEMICAL PHYSICS

**Head of the Department:**  
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### I. STAFF

**Full Professors:**

Fedor Valach, PhD, DSc

**Associate Professors:**

Pavol Fedorko, PhD, Oľga Holá, PhD, Viliam Laurinc, PhD, Peter Lukáč, PhD, Teodor Obert, PhD (part-time)

**Assistant Professors:**

Július Annus, Ladislav Bušovský, Eva Griačová (part-time), Juraj Griač, PhD (part-time), Soňa Halúsková (part-time), Vladimír Lukeš, PhD, Soňa Macková, PhD, Tibor Pálszegi, PhD (part-time), Vojtech Szócs, PhD (part-time), Miroslav Tokarčík, PhD, Daniela Žilinská

**Technical Staff:**

Anton Adamko, Marián Babnič, Zdenka Halaburková

### II. TEACHING AND RESEARCH LABORATORIES

#### A. Teaching Laboratories :

Laboratory of Physics I. (Mechanics, Deformations, Fluids, Heat)

Laboratory of Physics II. (Electrical measurements, DC and AC circuits, Waves, Black body radiation)

#### B. Research Laboratories:

Laboratory of X-ray Diffraction

Laboratory of Electrical Properties of Conducting Polymers

Laboratory of Gamma Radiation Source

### III. TEACHING

#### A. Undergraduate Study

1. Introductory Courses

**1st semester (autumn)**

|                          |        |   |
|--------------------------|--------|---|
| Seminar in Basic Physics | (0-2h) | Bušovský, Fedorko, Griačová, Holá, Halúsková, Laurinc, Lukáč, Lukeš, Macková, Obert, Tokarčík, Žilinská |
| Physics I.               | (2-2h) | Lukáč, Lukeš, Szócs   |

**2nd semester (spring)**

|                       |        |   |
|-----------------------|--------|---|
| Physics I.            | (2-2h) | Bušovský, Holá, Laurinc, Lukáč, Lukeš, Macková, Szócs, Tokarčík, Valach, Žilinská |
| Physics Laboratory I. | (0-2h) | Annus, Bušovský, Griačová, Griač, Halúsková, Lukeš, Macková, Tokarčík, Žilinská   |

**3rd semester (autumn)**

|                        |        |   |
|------------------------|--------|---|
| Physics II.            | (2-2h) | Bušovský, Fedorko, Holá, Laurinc, Macková, Tokarčík, Žilinská                   |
| Physics Laboratory II. | (0-2h) | Annus, Griač, Griačová, Halúsková, Lukeš, Macková, Pálszegi, Tokarčík, Žilinská |

2. Advanced Courses

**6st semester (spring)**

|                   |        |       |
|-------------------|--------|-------|
| Semestral project | (0-4h) | Lukeš |
|-------------------|--------|-------|

**8th semester (spring)**

|                            |        |                |
|----------------------------|--------|----------------|
| Statistical Thermodynamics | (2-1h) | Laurinc, Lukeš |
|----------------------------|--------|----------------|

### IV. CURRENT RESEARCH PROJECTS

#### A. Effect of gamma- and/or laser irradiation on the structure and critical temperature of copper-oxygen and fulleroid high-temperature superconductors as single crystals (Fedor Valach)

1. X-ray structure investigation of gamma- and/or laser irradiated single crystals of  $\text{La}_x\text{Sr}_{1-x}\text{CuO}_{2+\delta}$  and  $\text{C}_{60}$
2. Evaluation of the correlations of structural parameters versus critical temperature for high-temperature superconductors
3. Bond-valence approach to the copper-copper and copper-oxygen bonding in binuclear copper(II) complexes

4. X-ray crystallographic investigation of the temperature induced copper-oxygen isomers as single crystals

### **B. Theoretical study of thermo- and photochromism of thiophene based polymers (Viliam Laurinc)**

Common project with partners from the Dept. of Organic Chemistry, Slovak Academy of Sciences, and Institute of Chemistry at the Comenius University. The main goal of the project is the analysis of optical absorption and luminescence data obtained for variety of synthesised new thiophene oligomers and polymers. The quantitative trends of changes in optical properties are analysed by using the methods of quantum chemistry and theoretical simulations.

### **C. Optimization of didactic methods in physics (Oľga Holá)**

1. Formation of examination tests, use of microcomputer sets in the physical laboratory and introduction of interactive educational computer programmes
2. Pedagogico-psychologic-sociologic investigation of the motivation and social conditions of university students

## **V. COOPERATION**

### **A. Cooperation in Slovakia:**

Faculty of Electrical Engineering and Information Technology, Slovak University of Technology, Bratislava  
 Faculty of Mathematics and Physics, Comenius University, Bratislava  
 Faculty of Civil Engineering, Slovak University of Technology, Bratislava  
 Institute of Physics, Slovak Academy of Sciences, Bratislava  
 Institute of Polymers, Slovak Academy of Sciences, Bratislava  
 Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava  
 Faculty of Natural Science, Comenius University, Bratislava  
 VÚJE a.s., Trnava

### **B. International Cooperation:**

Institut für Festkörperphysik, Universität Wien, Vienna, Austria  
 - Fullerene and conducting polymer research  
 Institut für Physikalische Chemie, Universität Wien, Vienna, Austria  
 - Electronic excitation transport in polymers  
 Department of Inorganic Chemistry, Charles University, Prague, Czech Republic  
 - Synthesis of Co complexes  
 Institute of Chemistry, University of Wrocław, Wrocław, Poland  
 - X-ray crystallographic research  
 Laboratorium für Chemische und Mineralogische Kristallographie, Universität Bern, Bern, Switzerland  
 - X-ray crystallographic research  
 Department of Materials Science and Metallurgy, University of Cambridge, Cambridge, UK  
 - Electron diffraction research  
 Universidad de la Laguna, Tenerife, Spain  
 - Structural crystallophysics  
 Institut für Mineralogie, Technische Universität Wien, Vienna, Austria  
 - Crystallographic and structural chemistry  
 Chemical Crystallography Laboratory, Oxford University, Oxford, UK  
 - X-ray crystallographic research at low temperatures, crystallographic statistics  
 Nuclear Research Institut, Řež u Prahy, Czech Republic  
 - Emanation thermal analysis  
 Aristotle University, Thessaloniki, Greece  
 - Natural sorbents - zeolites  
 Departement de Recherche Fondamentale sur la Matière Condensée, Commissariat à l'Energie Atomique, Grenoble, France  
 - Conducting polymers

### **C. Membership in Domestic Organizations and Societies**

|   |   |
|---|---|
| Union of Slovak Mathematicians and Physicists, Bratislava | (V. Bušovský, P. Fedorko, O. Holá, V. Laurinc, S. Macková, T. Obert)            |
| Slovak Physical Society, Bratislava                       | (V. Bušovský, P. Fedorko, O. Holá, V. Laurinc, S. Macková, T. Obert, F. Valach) |
| Slovak Chemical Society, Bratislava                       | (F. Valach)   |

### **D. Membership in International Organizations and Societies**

|   |  |
|---|--|
| International Society for Theoretical Chemical Physics, Erlangen, Germany | (V. Laurinc)                               |
| European Synchrotron Radiation Society, Paris, France                     | (F. Valach)                                |
| European Physical Society, Budapest, Hungary                              | (P. Fedorko, O. Holá, T. Obert, F. Valach) |

### **H. Visits of Staff Members and Postgraduate Students in Foreign Institutions**

|            |   |
|------------|---|
| P. Fedorko | Departement de Recherche Fondamentale sur la Matière Condensée, Commissariat à l'Energie Atomique, Grenoble, France (since 3.12.2001) |
|------------|---|



## VII. PUBLICATIONS

### A. Journals (\*registered in Current Contents)

- [1]\* Valach F., Tokarčík M., Saunders A., Cowley A., Watkin D.J.: Structural isomerism of propionato copper(II) complex: crystal and molecular structure of tetrakis(m-o-propionato)bis(methyl 3-pyridyl-N-carbamate)dicopper(II) at 190 K. *Polyhedron* 20, 1933-1937 (2001)
- [2]\* Valach F., Tokarčík M., Maris T., Watkin D.J., Prout C.K.: Bond-valence approach to the copper-copper and copper-nitrogen bonding in binuclear copper(II) complexes: Structure of tetrakis(2-iodobenzoato)bis(caffeine)dicopper(II) at 210 K. *J. Organomet. Chem.* 622, 166-171 (2001)
- [3]\* Lukeš V., Vrabel I., Laurinc V., Biskupič S.: Ab initio study of the Li-H<sub>2</sub> van der Waals complex. *Chem. Phys.* 271, 1-8 (2001)
- [4]\* Lukeš V., Vrabel I., Laurinc V., Biskupič S.: Ab initio study of the HF-H van der Waals complex. *J. Phys. Chem. A* 105, 7686-7692 (2001)
- [5]\* Lukeš V., Breza M., Pálszegi T., Laurinc V., Vrabel I.: On the relation between conformational changes and optical properties in oligothiophenes. 2. Linear and nonlinear optical properties. *Macromol. Theory Simul.* 10, 592-599 (2001)
- [6]\* Lukeš V., Breza M., Végh D., Hrdlovič P., Krajčovič J., Laurinc V.: Non-linear optical properties of new bridged bis-thienyls. I. Pyrazine-based bridges: theory, synthesis and spectra. *Synthetic Metals* 124, 279-286, (2001). *Simul.* 10, 592-599 (2001)
- [7]\* Breza M., Lukeš M., Vrabel I.: On the dependence of optical properties on conformational changes in oligothiophenes. I. Electron absorption spectra. *J. Mol. Struct. (THEOCHEM)* 572, 151-160 (2001)
- [8]\* Fedorko P., Fraysse J., Dufresne A., Planés J., Travers J. P., Olinga T., Kramer C., Rannou P., Pron A.: New counterion-plasticized polyaniline with improved mechanical and thermal properties: comparison with PANI-CSA. *Synthetic Metals* 119, 445-446 (2001)
- [9]\* Tkáč J., Voštiar I., Šturdík E., Gemeiner P., Mastihuba V., Annus J.: Fructose biosensor based on D-fructose dehydrogenase immobilised on a ferrocene-embedded cellulose acetate membrane. *Anal. Chim. Acta* 439, 39-46 (2001)
- [10]\* Dufour B., Rannou P., Fedorko P., Djurado D., Travers J.-P., Pron A.: Effect of plasticizing dopants on spectroscopic properties, supramolecular structure, and electrical transport in metallic polyaniline. *Chem. Mater.* 13, 4032-4040 (2001)
- [11] Vial J.-C., Pépin-Donat B., Viallat A., Fedorko P.: Carrier dynamics in poly(octylthiophene) gels. *Mat. Res. Soc. Symp. Proc.* 660, JJ8.22.1-JJ8.22.6, (2001)

### B. Conferences (\*international conferences)

- [1]\* Holý K., Ridziková A., Polášková A., Stanys T., Bosá I., Holá O.: Temporal variability of some radon characteristics of the soil. In: Proc. XXIV. Days of Radiation Protection, Demänovská dolina, Slovakia, Nov. 26.-29. 2001, p.68-73
- [2]\* Holý K., Patschová E., Holá O., Bosá I., Polášková A.: Detection system for continuous <sup>222</sup>Rn monitoring in waters. In: Proc. XXIV. Days of Radiation Protection, Demänovská dolina, Slovakia, Nov. 26.-29. 2001, p.65-67
- [3]\* Földešová M., Dillinger P., Lukáč P.: Studies of adsorption of zinc ions on zeolites by means of Zn-65. In: Proc. XXIV. Days of Radiation Protection, Demänovská dolina, Slovakia, Nov. 26.-29. 2001, p.27-31
- [4]\* Valach F., Tokarčík M., Maris T., Saunders A., Cowley A., Watkin D.J., Prout C.K.: Prediction of metal-ligand bond length in copper complexes using bond-valence model. In: Proc. 18. Int. Conf. on Coordination and Bioinorganic Chemistry, Smolenice, Slovakia, June 4.-8. 2001, p.68
- [5]\* Holý K., Matoš M., Stanys T., Holá O., Polášková A., Bosá I.: Testing of the <sup>222</sup>Rn as a tool for determination of CO<sub>2</sub> exhalation rates from the soil. In: Banská Štiavnica, Slovakia, Oct. 6.-7. 2000, p.124-138
- [6] Holá O., Laurinc V.: Systém kontroly vedomostí z fyziky. In: Zborník z 2. odb. seminára: Náplň a poslanie fyziky na I. stupni VŠ vzdelávania a nové vzdelávacie technológie na VŠ technických (in Slovak). Trnava, Slovakia, May 31. 2001, p. 54-61
- [7] Laurinc V., Holá O.: Fyzika na CHTF STU-súčasnosť a budúcnosť. In: Zborník z 2. odb. seminára: Náplň a poslanie fyziky na I. stupni VŠ vzdelávania a nové vzdelávacie technológie na VŠ technických (in Slovak). Trnava, Slovakia, May 31. 2001, p. 49-53
- [8]\* Dufour B., Rannou P., Djurado D., Fedorko P., Pron A.: Polyaniline metallique aux proprietes mecaniques ameliores: preparation, structure et proprietes de transoport. In: 9. Journées Polymères Conducteurs, Angers, France, Sept.18.-21. 2001, p.C03-06
- [9]\* Fedorko P., Djurado D., Genoud F., Dufour B., Pron A., Rannou P., Travers J.P.: Vieillessement thermique vs vieillissement sous irradiation: nouvelle évidence en faveur de l'hétérogénéité dans la polyaniline. 9. Journées Polymères Conducteurs, Angers, France, Sept.18.-21. 2001, p.P3-15
- [10]\* Pépin-Donat B., Vial J.-C., Viallat A., Fedorko P.: Dynamique des porteurs de charges dans les gels de poly(octylthiophene) gonflés. 9. Journées Polymères Conducteurs, Angers, France, Sept. 18.-21. 2001, p. P3-09.
- [11]\* Szócs V., Pálszegi P., Lukeš V., Tortschanoff A. and Kauffmann H.F.: Excitonic coupling in bichromophoric molecules: structural information from 2D two-pulse photon echoes - a theoretical study. In: 5th Femtochemistry conference, Toledo, Spain, Sept. 2.-6. 2001, p. P117-P118
- [12]\* Lukeš V., Laurinc V., Biskupič S., Vrabel I.: Ab initio štúdium van der waalsovských komplexov. Plocha potenciálnej energie komplexu Li-H<sub>2</sub>. In: XII. Konferencia slovenských fyzikov, Smolenice, Slovakia, Sept. 3.-9. 2001, p.119-120
- [13]\* Valach F., Tokarčík M., Maris T., Saunders A., Cowley A., Watkin D.J., Prout C.K.: Application of bond-valence theory to structures of coordination compounds. In: Materials Structure in Chemistry, Biology, Physics and Technology. Bedřichov, Czech Republic, June 18.-22. 2001, p.19-20

### C. Books and Textbooks

- 1] Holá O., Veselský J., Baník I., Machovič L., Macáková M., Tomčík P., Valková M., Minárik S., Labaš V.: Príručka k prijímacím skúškam z fyziky na STU v Bratislave (in Slovak). STU Bratislava, 69 pp. (2001)

### E. Others:

- [1] Laurinc V., Holá O.: Mechanika tekutín. Kapitola v internetovej učebnici fyziky v rámci Internet Distance Education Program (in Slovak). Internet Program IDEP, (2001)

## DEPARTMENT OF CHEMICAL TECHNOLOGY OF WOOD, PULP AND PAPER

Head of the Department:  
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### I. STAFF

#### Associate Professors:

Svetozár Katuščák, PhD, Pavel Krkoška, PhD, Ladislav Šutý, PhD

#### Assistant Professors:

Vlasta Lužáková, PhD, Pavel Mišovec, PhD, Štefan Šutý, PhD, Katarína Vizárová, PhD

#### Research Fellows:

Tatiana Marcinčinová, Igor Šurina, PhD, Milan Vrška, PhD

#### PhD Students:

Andrea Barteková, Rudolf Dorko, Gabriela Szeiffová, Radovan Tiňo

#### Technical Staff:

Jozefína Karabová, Valéria Törökóvá, Ivan Vajanský, Zuzana Žaškovská

### II. TEACHING AND RESEARCH LABORATORIES

#### A. Teaching Laboratories:

Laboratory of Wood Structure and Analysis  
Laboratory of Chemical Treatment of Wood  
Laboratory of Pulping Technology  
Laboratory of Papermaking Fibres and Additives

#### B. Research Laboratories

Laboratory of Wood Chemistry  
Laboratory of Structure and Properties of Paper  
Laboratory of Natural Polymers  
GC-MS Laboratory

### III. TEACHING

#### A. Undergraduate Study

##### 6th semester (spring)

|                    |         |                       |
|--------------------|---------|-----------------------|
| Semestral Project  | (0-4 h) | members of department |
| Paper and Printing | (2-2 h) | P. Krkoška, J. Panák  |

##### 7th semester (autumn)

|   |         |                          |
|---|---------|--------------------------|
| Physics of Polymers and Paper                       | (2-2 h) | M. Krištofič, Š. Šutý    |
| Wood Chemistry and Analysis                         | (2-0 h) | S. Katuščák, K. Vizárová |
| Pulping Technology                                  | (3-1 h) | M. Vrška, Š. Šutý        |
| Laboratory  | (0-8 h) | K. Vizárová              |
| Natural Polymers                                    | (2-1 h) | V. Lužáková, D. Bakoš    |
| Environmental Management in Pulp and Paper Industry | (2-0 h) | K. Vizárová, S. Katuščák |

##### 8th semester (spring)

|                                |         |                                 |
|--------------------------------|---------|---------------------------------|
| Paper Technology I.            | (3-0 h) | P. Krkoška, Š. Šutý             |
| Paper Machines                 | (2-2 h) | A. Čerňanský                    |
| Engineering of Pulp Production | (1-1 h) | L. Šutý, M. Vrška               |
| Chemical Treatment of Wood I.  | (3-0 h) | I. Šurina, S. Katuščák          |
| Laboratory                     | (0-8 h) | M. Vrška, I. Šurina, P. Mišovec |

##### 9th semester

|  |         |                                 |
|--|---------|---------------------------------|
| Chemical Treatment of Wood II.           | (2-0 h) | I. Šurina, Š. Šutý              |
| Paper Technology II.                     | (3-0 h) | P. Krkoška, P. Mišovec          |
| Packaging Materials                      | (2-0 h) | P. Mišovec                      |
| Laboratory                               | (0-9 h) | M. Vrška, I. Šurina, P. Mišovec |
| Chemical Aids in Pulp and Paper Industry | (1-1 h) | V. Lužáková, K. Vizárová        |

**10th semester (spring)**

Thesis 0-27 h supervisors

**PhD Study**

Technology of polymeric materials 12 months P. Krkoška

**IV. CURRENT RESEARCH PROJECTS****A. Papermaking fibres-new process of isolation, modification, recyclation and preparing of paper (Pavel Krkoška)**

The project respects the request of Slovak industry of chemical treatment of wood, and chemical technology of pulp and paper. Definition and mathematical description of pulp fibres properties by new delignification and bleaching processes in laboratory and industrial conditions, definition of their permanence and durability was studied. The database of monitoring of emission from pulp and paper industry of Slovak Republic was verified. The analysis of wood raw materials with regard to the content of calcium was studied.

**B. Thermal degradation of plant cell wall polysaccharides (Ivan Šimkovic, Igor Šurina)**

Thermal degradation of wood cell wall polysaccharides and the possibilities of retarding this process were studied. This can be achieved by impregnation of wood materials with appropriate mixtures and by subsequent precipitation of the formed products in the cell wall by acidification. The identification of compounds formed by thermolysis of starch and their derivatives was accomplished also by GC/MS methods.

**C. Interaction of Nonprocess Components Under Pulping Condition (Vlasta Lužáková)**

Yield and composition of the lipophilic wood extractives of the twelve domestic wood species have been studied by solvent extraction of the wood samples followed by fractionation of the isolated extractives using SPE, and the two pitch formation precursors, originated from wood, were evaluated. The calcium content, determined in the ashed wood samples by AAS, was evaluated as the third pitch formation precursor.

Chosen lipophilic fractions in the pulp treated with anti-deposit agents, the mixture of surfactants or an inorganic adsorbent, have been quantitatively analyzed.

An analytical procedure convenient for the determination of sterol structures present in the mixture of isolated lipophilic wood extractives was developed when appropriate chemical standards, the derivative agents and procedures, as well as GC-MS analysis were employed for that purpose.

**D. New methods of valorisation of wood with regards to finalisation and environment protection (Svetozár Katusčák)**

Research and development of competitive technologies and products in the woodworking area. Analyses of the trends wood composite panels and furniture research and production. Literature. Laboratory preparation and testing of wood panels from PIR and PCR raw materials. Research of wood composites with environmental quality (EQ) close to natural wood. Study of the methods of quantifying of parameters characterising natural wood in regards to Interior Air Quality (IAQ). Proposal of the complex of characteristic parameters for quantifying EQ and image of wood composites from recycling in comparison with natural massive wood.

**E. Influence of papermaking processes on the paper roughness (Štefan Šutý)**

The aim of this work was identified the processes on the paper machine which influenced the paper roughness. From the literature was identified the processing parameters influenced on the paper roughness. The influence of the processing parameters was verified using the multivariable regression with statistical calculation of the significance of the parameters.

**V. COOPERATION****A. Cooperation in Slovakia**

North Slovakian Pulp and Paper Company, Ružomberok  
Pulp and Paper Research Institute, Bratislava  
State Forest Products Research Institute, Bratislava  
Institute of Wood Ecology, Nitra  
Technical University, Zvolen  
Slovak National Archives, Bratislava  
Institute of Chemistry of Slovak Academy of Sciences, Bratislava  
Bukóza Co., Vranov  
AssiDomán Packaging, Štúrovo; Kappa Štúrovo a.s.  
Union of Pulp and Paper Industry of Slovak Republic, Banská Bystrica  
Institute of Forest Ecology, Zvolen

**B. International Cooperation**

Department of Chemical Technology of Wood, Pulp and Paper, Technical University, Pardubice, Czech Republic  
- Pulp and Paper Chemistry and Technology  
Czech State Central Archives, Praha, Czech Republic  
- Permanence and Durability of Paper  
Leopold-Franzens University, Innsbruck, Austria  
- Properties of Fibers from TMP  
Institute of Papermaking and Paper Machines, Technical University of Lodz, Poland  
- Cooperation in Pedagogical and Research Activities

University of Quebec - Trois Rivières, Canada  
 - Properties of Explosion Pulp  
 Pulp and Paper Research Centre, McGill University, Montreal, Canada  
 - Filling of Paper  
 Agricultural University, Faculty of Wood Technology, Poznan, Poland  
 - Chemical Techn. of Wood and Plant Raw Materials  
 University of Provence, Marseille, France  
 - Combustion  
 French Institute of Papermaking and Graphics Industry, Grenoble, France  
 - Pulp and Paper Chemistry and Technology  
 Universidade da Beira Interior, Covilhã, Portugal  
 - Program Socrates

### C. MEMBERSHIP IN DOMESTIC ORGANIZATIONS AND SOCIETIES

Slovak Chemical Society, Bratislava (P: Krkoška, I. Šurina, L. Šutý)  
 Slovak Society of Industrial Chemistry, Bratislava (P. Krkoška, V. Lužáková, P. Mišovec, I. Šurina)  
 SK-Biom, Bratislava (I. Šurina)  
 Union of Pulp and Paper Industry of Slovak Republic, Banská Bystrica (P. Krkoška, L. Šutý, Š. Šutý)

### D. MEMBERSHIP IN INTERNATIONAL ORGANIZATION AND SOCIETIES

TAPPI - Technical Association of the Pulp and Paper Industry, Atlanta, USA (P. Krkoška)  
 Society of the Pulp and Paper Industry, Prague - Bratislava, Czech and Slovak republic (I. Šurina)

### E. TEMPUS PROGRAM

### F. INTERNATIONAL SCIENTIFIC PROGRAMS

### G. VISITORS FROM ABROAD

Prof. M. Milichovský Technical University, Pardubice, Czech Republic, June and September, (4 days)  
 Prof. B. Alince McGill University, Montreal, Canada, September 2001, (3 days)  
 Prof. W.Z.Tarnawski Technical University of Lodz, Institute of Papermaking and Printing Technology, Poland, September 2001, (2 days)  
 Wei Shen, PhD Australian Pulp and Paper Institute, Department of Chemical Engineering, Australia, December 2001, (1day)  
 Rogut R., PhD Technical University of Lodz, Poland, September 2001, (2 days)  
 Prof. B. Kokta University of Quebec - Trois Rivières, Canada (2 days)

### H. VISITS OF STAFF MEMBERS AND PHD STUDENTS IN FOREIGN INSTITUTIONS

Szeiffová G. McGill University, Montreal, Canada, December 2001  
 Buchtová A. Faculty of Science of University Porto, Portugal, May (30 days)

### VI. THESES AND DISSERTATIONS

#### A. Undergraduate Theses (BSc Degree) for state examinations after three years of study (supervisors are written in brackets):

Balontayová S.: Influence of additives on strength properties of paper (Mišovec P.)  
 Coková A.: Permanence and durability of hand made papers destined to restoration (Krkoška P.)  
 Černáková S.: Influence of elektrokinetics properties of components of papermaking suspension to the retention of the filler (Šutý S.)  
 Gorelková T.: Verification of New Methods of Objective Evaluation of the Surface Resistance of Laminated Particleboards (Katuščák S.)  
 Hajdamárová I.: Nonchlorine bleaching compounds in bleaching of low Kappa pulps (Vrška M.)  
 Husárik M.: Pulp structure changes by accelerated ageing (Vizárová K.)  
 Kerekeš J.: Interaction of lipophilic wood extractives and pitch controlling agents (Lužáková V.)  
 Kolláriková A.: Influence process waterflow on final parameters of chemical and biological oxygene consumption (Helcman)  
 Miková G.: The evaluation of the emission of volatile organic compounds from

|               |  |
|---------------|--|
| Nemčeková A.: | lignocellulose materials (Katuščák S.)   |
| Pengerová V.: | Composite properties of materials made from pulp fibres and synthetic latexes (Tiňo R.)                    |
| Tešlárová B.: | Optimization of process parameters at adsorptive core formation of Pantyliner with addition of SAP (Palka) |
|               | Bonding ability of recycled fibers from waste paper (Mišovec P.)   |

**B. Graduate Theses (MS Degree)****C. Dissertations (PhD)****VII. PUBLICATIONS****A. Journals (\*registered in Current Contents, CA and in ABIPST)**

- [1]\* Fišerová M., Lužáková V.: Application of Surfactans as Kraft Pulping Additives. Bulletin PPRI, Bratislava, Vol.36, 1, 1-17 (2000)
- [2] Katuščák S.: Photo – induced modification of the optical properties of lignocellulose materials. Effect of substrate surface on the photoyellowing of surface – coated lignin model compounds. In.: Drevársky výskum 45 (2) :1 – 14, 2000 (Published in 2001)
- [3] Katuščák S., Kučera L.J.: Cie orthogonal and cylindrical color parameters and the color sequences of the temperate wood species. In.: Drevársky výskum 45 (3): 9 – 22, 2000 (Published in 2001)
- [4]\* Marcinčin A., Jurčišinová Z., Borsig E., Krištofič M., Marcinčinová T.: Fiberforming Blend Polypropylene – Polyvinyl Alcohol. Polymers for Advanced Technologies, 12, 2001, 1-5

**B. Conferences (\*international conferences)**

- [1] Buchtová A., Šurina I., Katuščák S., Miková G., Vrška M.: Vplyv prchavých organických látok (VOC) na ľudské zdravie. Influence of VOC on human health (in Slovak). In: Proceedings of conference " Pulp and Paper – Technology, Properties, Environment", Bratislava 11.-12.september 2001, ISBN 80-227-1566-2, 34-40
- [2] Buchtová A., Ventura G., Martins A., Šurina I., Katuščák S.: Stanovenie emisií prchavých organických látok (VOC) pomocou FLEC (Field and Laboratory Emission Cell) - náhrada komorovej metódy. Determination of VOC emissions by FLEC (Field and Laboratory Emission Cell) (in Slovak). In: Proceedings of conference " Pulp and Paper – Technology, Properties, Environment", Bratislava 11.-12.september 2001, ISBN 80-227-1566-2, 233-235
- [3] Hanus J., Coková A., Krkoška P.: Niektoré historické a súčasné ručné papiere z hľadiska stálosti a trvanlivosti. Permanence and durability of some historical and present handmade papers (in Slovak). In: Proceedings of conference " Pulp and Paper – Technology, Properties, Environment", Bratislava 11.-12.september 2001, ISBN 80-227-1566-2, 206-210
- [4] Kerekeš J., Lužáková V., Šurina I.: Analýza sterolových štruktúr v zmesi lipofilných extaktívnych látok dreva. Analysis of Sterol Structures in the Mixture of Lipophilic Wood Extractives (in Slovak). In: Proceedings of conference " Pulp and Paper – Technology, Properties, Environment", Bratislava, 11. - 12. September 2001, ISBN 80-227-1566-2, 227-232
- [5] Krkoška P., Tiňo R.: Číselný opis papierenských vlastností buničínových vlákien. Numerical description of papermaking properties of pulp fibers ( in Slovak). In: 53.Zjazd chemických spoločností 3.-6. september 2001, Banská Bystrica, Zborník príspevkov ISBN 80-89029-23-X C-P1, 221-224, (in Slovak)
- [6] Krkoška P., Vizárová K.: Stálosť a trvanlivosť niektorých buničín a papierov. Permanence and durability of some pulps and papers (in Slovak). In: Proceedings of conference " Pulp and Paper – Technology, Properties, Environment", Bratislava 11.-12.september 2001, ISBN 80-227-1566-2, 171-178
- [7] Lužáková V.\*, Marcinčinová T., Šutý Š.: Možnosti využitia merania náboja povrchu častíc vo výrobe buničiny a papiera. Possibilities of the Particle Charge Determination Usage in Pulp and Paper Production (in Slovak). In: 53. Zjazd chemických spoločností, 3.-6. September 2001, Banská Bystrica, Zborník príspevkov ISBN 80-89029-23-X C-P5, 230-231
- [8] Marcinčin A., Legéň J., Hudecová D., Marcinčinová T., Šesták J., Spevárová E.: Antibacterial Chemical Fibres and Fibrous Materials. 1<sup>st</sup> AUTEX Conference TECNITEX 2001, Technical textiles, Designing Textiles for Technical Applications, Povoa de Varzim, University of Minko, Portugalsko, 27<sup>th</sup> and 28<sup>th</sup> June 2001.
- [9] Marcinčin A., Legéň J., Marcinčinová T.: Antibacterial Viscose Fibres. In: Proceedings of 2<sup>nd</sup> Central European Conference on Fibro-Grade Polymers, Chemical Fibres and special Textiles (CEC Monograph series Vol 2), Slov. Univ. of Technol., Bratislava 2001, 239-243.
- [10] Marcinčin A., Ujhelyiová A., Hricová M., Marcinčinová T.: Modification of Polypropylene Fibres by Polymeric Additives. International Millenium Congress on Inovations in Fibre , Jam Fabric Technology and Finishing. Terrassa, Španielsko, 2001.
- [11] Marcinčin A., Ujhelyiová A., Zemanová E., Marcinčinová T.: Mass pigmenting of polypropylene and polyethylene terephthalate fibres. In: Fibro-Grade Polymers, Chemical Fibres and special Textiles (Struszczyk H., Marcinčin A., Wlochovycz A. Eds) 1<sup>nd</sup> Central European Conference Monograph Series. Lodz, Poland 2001, Vol 1, 145-155
- [12] Marcinčin A., Zemanová E., Marcinčinová T., Brejka O., Budzák D.: Rheological Properties of Polyester Pigment Concentrates. In: Proceedings of 2<sup>nd</sup> Central European Conference on Fibro-Grade Polymers, Chemical Fibres and special Textiles (CEC Monograph series Vol 2), Slov. Univ. of Technol., Bratislava 2001, 239-243.
- [13] Mišovec P.: Vázbová schopnosť recyklovaných vlákien zo zberového papiera. Bonding ability of recycled fibers from waste paper (in Slovak). In: Proceedings of conference " Pulp and Paper – Technology, Properties, Environment", Bratislava 11.-12.september 2001, ISBN 80-227-1566-2, 146-149
- [14] Mišovec P.: Vplyv aditív na väzobnú schopnosť vlákien. Influence of additives on bonding ability of pulp fibres (in Slovak). In: 53.Zjazd chemických spoločností 3.-6. september 2001, Banská Bystrica, Zborník príspevkov ISBN 80-89029-23-X, C-P7, 234-235
- [15] Šutý Š., Bieliková L., Bednár F., Tiňo R., Buchtová A.: Účinnosť zrážok - parameter na predpovedanie retencie plniva v papieri. Collision efficiency the parameter for prediction the retention of the filler in the paper (in Slovak). In: Proceeding of conference " Pulp and Paper – Technology, Properties, Environment", Bratislava 11.-12.september 2001, ISBN 80-227-1566-2, 136-141

- [16] Šutý Š., Majlenderová Z., Tiňo R.: Zmena veľkosti častíc flokuláciou indukovanou polyelektrolytom v procese plnenia papiera. Change of particle size by polyelectrolyte induced flocculation in the process of filling the paper (in Slovak). In: Proceedings of conference " Pulp and Paper – Technology, Properties, Environment", Bratislava 11.-12.september 2001, ISBN 80-227-1566-2, 142 – 145
- [17] Šutý Š., Szombathová A.: Použitie prírodných zeolitov ako plniva do papiera. Using the natural zeolites as a filler to the paper (in Slovak). In: 53.Zjazd chemických spoločností 3.-6. september 2001, Banská Bystrica, Zborník príspevkov ISBN 80-89029-23-X, C-P4, 228-229
- [18] Tiňo R., Alince B.: Modelový systém sledovania depozície latexových častíc a vytvorenia latexovej viacvrstvy. Model systém of following of the latex particles deposition and creation of latex multilayers (in Slovak). In: Proceedings of conference " Pulp and Paper – Technology, Properties, Environment", Bratislava 11.-12.september 2001, ISBN 80-227-1566-2, 150-154
- [19] Vizárová K.: Starnutie papiera a zmena farby. Ageing of paper and colour changes (in Slovak). In: 53. Zjazd chemických spoločností 3.-6. september 2001, Banská Bystrica, Zborník príspevkov ISBN 80-89029-23-X, C-P8, 236-237
- [20] Vrška M., Šurina I.: Vápnik – trvalý problém pri výrobe buničín. Calcium - a Permanent Problem in Pulping Technology (in Slovak). In: Proceedings of conference " Pulp and Paper – Technology, Properties, Environment", Bratislava 11.-12. september 2001, ISBN 80-227-1566-2, 64-68.

### C. Books and Textbooks

### D. Patents

### E. Others

- [1] I. Šurina, PhD.: FChPT Project 10/01, EBA,s.r.o.
- [2] I. Šurina, PhD.: FChPT Project 11/01, KAPPA Štúrovo a.s.
- [3] I. Šurina, PhD.: FChPT Project 40/01, KAPPA Štúrovo a.s.
- [4] V. Lužáková, PhD.: FChPT Project 43/01, SCP Ružomberok
- [5] I. Šurina, PhD.: FChPT Project 63/01, D.V.M.
- [6] I. Šurina, PhD.: FChPT Project 64/0, SCP Ružomberok
- [7] I. Šurina, PhD.: FChPT Project 84/01, KAPPA Štúrovo a.s.
- [8] Š. Šutý, PhD.: FChPT Project 86/01, SCP Ružomberok
- [9] Š. Šutý, PhD.: FChPT Project 101/01, Purgina, Bratislava
- [10] I. Šurina, PhD.: FChPT Project 118/01, Slovnaft, a.s., Bratislava
- [11] S. Katuščák, PhD., FChPT Project 125/01, KAPPA Štúrovo a.s.
- [12] I. Šurina, PhD.: FChPT Project 126/01, Jaroslav Samuhel
- [13] M. Vrška, PhD.: FChPT Project 140/01, Fellegi Techn. Consulting, Bratislava
- [14] S. Katuščák, PhD.: FChPT Project 152/01, MK
- [15] V. Lužáková, PhD.: FChPT Project 197/01, SCP Ružomberok

## DEPARTMENT OF ENVIRONMENTAL SCIENCES

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### I. STAFF

#### Full Professors:

Vasil Koprda, PhD, DSc, Juraj Tölgyessy, PhD, DSc

#### Associate Professors:

Marta Čerňáková, PhD, Gabriel Čík, PhD, Ján Derco, PhD, Pavel Dillinger, PhD, Miloslav Drtil, PhD, Margita Harangozó, PhD, DSc, Anežka Moncmanová, PhD (Assoc.Prof.Emer.), Milan Piatrik, PhD, Josef Prousek, PhD

#### Research Fellows:

Petra Bendová, Igor Bodík, PhD, Assoc.Prof. Agáta Fargašová, PhD, DSc, Mária Földesová, Miroslav Hutňan, PhD

#### PhD Students:

Juraj Buday, Eva Gašparíková, Angelika Gulyasová, Milada Hubinová, Zoltán Kassai, Lea Mrafková, Andrea Pálinkášová-Bujnová, Marek Horňák, **external form:** Petra Bendová, Alžbeta Ďurecová, Ladislav Halász, Angelika Kassai, Alexander Kovács, Rastislav Kuffa, Ladislav Maro, Jana Marová, Eva Mihalíková, Salima Shansab, Jana Želinská, Jana Vanečková-Pichová

#### Technical Staff

Eleonóra Hornáčková, Marta Onderová

### II. TEACHING AND RESEARCH LABORATORIES

#### A. Teaching Laboratories:

Laboratory of Water Chemistry  
Laboratory of Nuclear Analytical Chemistry

#### B. Research Laboratories:

Laboratory of Air Protection Technology  
Laboratory of Microbiology and Ecotoxicology  
Laboratory of Organic Chemistry  
Laboratory of Radioecology  
Laboratory of Water and Wastewater Technology  
Laboratory of Computer Modelling

### III. TEACHING

#### A. Undergraduate Study

##### 5th semester (autumn)

Nuclear Chemistry and Technology I. (1-1) Koprda, Dillinger

##### 6th semester (spring)

Environmental Technology (2-0) Piatrik, Čík, Koprda,

##### 7th semester (autumn)

Biology of Water, Soil and Air (2-0) Čerňáková, Fargašová  
Atmospheric and Water Chemistry (4-0) Prousek, Bodík  
Hydrology, Meteorology and Pedology (2-0) Fargašová, Čerňáková  
Laboratory Practice I. (0-8) Harangozó, Bodík, Dillinger, Fargašová,  
Földesová, Čerňáková  
Nuclear Chemistry and Technology II. (2-0) Koprda, Dillinger

##### 8th semester (spring)

Air Protection Technology (2-0) Čík, Prousek  
Laboratory Practice II. (0-8) Derco, Dillinger, Čík  
Radioecology (2-0) Harangozó, Dillinger  
Wastewater Engineering (2-2) Derco, Drtil

##### 9th semester (autumn)

Branch - Technology of Environment (2-0) Prousek, Čerňáková  
Risk Properties of Substances (0-10) Drtil, Harangozó, Čík  
Liquidation and Utilization of Solid Wastes (2-0) Piatrik, Koprda  
Environmental Technological Project (3-0) Drtil, Derco

|   |        |                          |
|---|--------|--------------------------|
| Environmental Impact Assessment             | (2-0)  | Koprda, Piatrik          |
| Control of Environmental Pollution          | (2-0)  | Harangozó, Dillinger     |
| Special Ecology and Ecotoxicology           | (2-0)  | Fargašová, Prousek       |
| Processes and Technology of Water Treatment | (3-0)  | Hutňan, Bodík            |
| Air Protection Technology and Air Treatment | (3-0)  | Čík, Prousek             |
| <b>10th semester (spring)</b>               |        |                          |
| Diploma Work                                | (0-30) | all members of the staff |

## B. PhD Study

### 1. Environmental Chemistry and Technology

|   |       |               |
|---|-------|---------------|
| Anaerobic Wastewater Treatment Processes                        |       | Derco, Hutňan |
| Progressive Methods of Wastewater Treatment                     |       | Derco, Drtil  |
| Combination of Anaerobic-aerobic Wastewater Treatment Processes | Bodík |               |
| Simulation of Biological Processes of Wastewater Treatment      |       | Derco         |
| Utilization of Ozone for Wastewater Treatment                   |       | Derco         |

### 2. Nuclear Chemistry and Radioecology

|  |  |                   |
|--|--|-------------------|
| Penetration of Radionuclide across Skin Barriers           |  | Koprda, Harangozó |
| Study of Metal Transport from Abiotic to Biotic Systems    |  | Koprda, Lesný     |
| Effect of Aerosol Size Fractions on Health Risk Assessment |  | Koprda            |
| The Use of Fenton Reaction to Wastewater Treatment         |  | Koprda, Prousek   |

## IV. CURRENT RESEARCH PROJECTS

### A. The study of separation and immobilisation of radionuclides from nuclear power cycle by natural adsorbers (Pavel Dillinger)

The determination of sorption capacity of chemically modified natural zeolites towards some cations was studied by static radioexchange and AAS methods. It was studied the sorption of Sn(II), Zn(II), Cs(I) and Co(II). Radionuclides Sn-113, Zn-65, Cs-137 and Co-60 were used as radiotracers. The dependence of structure, sorption capacity and the desorption of natural and chemically modified zeolites for individual cations on pH, temperature and competitive cations (Cr, Zn, Ca, Cu, Fe, Cs, Co) was studied. All these parameters were studied on model water solutions labelled by radionuclides. The sorption of Sn from two chemical different solutions  $\text{SnCl}_2$  and  $\text{SnCl}_4$  was studied. It was studied the sorption of cations from mixed solutions (Cs + Co) by new types of natural and chemically modified sorbents (zeolite, mordenite, bentonite smectite, clays). We demonstrated that the sorption capacity of natural and chemically modified sorbents depend not only on these materials but also on the chemical properties of studied solutions and pH. The results of our research were presented in journals and in international conference XXIV. Days of radiation protection.

Determination of copper, cesium, selenium and other heavy metals in ashes from fy Duslo Šála by radionuclide X-ray fluorescence technique was done. Heavy metals Cu, Fe, Pb and Zn were determined in agricultural refine plants (cereals) by AAS method.

It was developed the high-senzitive detection system for continuous Rn-222 monitoring in waters. The device can be used for the continual control of radon activity concentration in water sources, the daily and seasonal variations of radon activity in water systems and for the determination of the infiltration time of surface water into the ground water. The time variability of the volume activity of Rn-222 in the various depth of the soil and the radon exhalation's rate from the soil surface were studied.

### B. Progressive Methods of Water, Wastewater and Activated Sludge Treatment (Ján Derco)

1. Utilisation of ozone for removal of biorefractory organics (J. Derco, A. Gulyášová)

The effectiveness of ozone treatment for improvement of the biodegradability of biorefractory organic pollutants contained in a landfill leachate after biological pre-treatment was also studied. Contaminants transformation was monitored by means of overall parameters related to the concentration of organic compounds in the treated samples, i.e., chemical oxygen demand (COD) and biochemical oxygen demand (BOD). Approximately 60 % reduction of COD in biologically pre-treated landfill leachate was observed after about 10 to 11.5 h lasting ozonation. Maximum observed  $\text{BOD}_5$  value, measured by respirometric method was  $244 \text{ mg dm}^{-3}$ . Biodegradability expressed as  $\text{BOD}_5/\text{COD}$  ratio increased from zero up to a maximum value of 0.21, corresponding to the ozone consumption of 0.7 mg per mg of reduced COD.

2. Municipal wastewater treatment in anaerobic and aerobic reactors at low temperature (I. Bodík, E. Gašpariková)

The low temperature influence (5-25 °C) on the municipal wastewater treatment processes under anaerobic conditions has been studied. The reduction of the reactor volume and operational costs and determination of optimum combination of anaerobic and aerobic reactors for municipal wastewater treatment plants were the aim of research. The experiments with the real wastewater on the pilot-scale reactor on the wastewater treatment plants in Bratislava were realised.

3. Toxicity, accumulation and interactions of metals in water and terrestrial organisms (A. Fargašová)

During the tests the attention was dedicated to the effects and bioaccumulation of metals and their reciprocal interactions for selected freshwater benthic and plankton organisms and some terrestrial plants. For determination of metal accumulation in alga cells and plant roots and cotyledones the analytical methods AAS and RXFA were used. The obtained results help to solve problems connected with metal removing from the environment and to establish the limit values for some metals.

4. Anaerobic waste and wastewater treatment processes and technologies (M. Hutňan, M. Drtil, M. Horňák)

Laboratory experiments with anaerobic treatment of selected organic wastes have been realised. Experiments were carried out with sugar beet pulp as a by-product of sugar production and with grain distillery slops. Possibilities of the start-up of the sugar beet pulp anaerobic treatment with various types of inoculum were observed and compared. Aerobic treatment of sludge water from the



anaerobic treatment of sugar beet pulp was studied, too. From this research very good anaerobic degradation of the sugar beet pulp resulted. High efficiency of organic carbon and nitrogen removal during sludge water aerobic treatment was achieved. Grain distillery slops are interesting material for anaerobic treatment. They contain much more proteins as other types of the stillages (from molasses, fruits etc.). Therefore, different conditions of anaerobic degradation and different quality of sludge water can be assumed. From this point of view the process was studied. In addition, anaerobic processes and odour formation in sewer system were studied, too. Research was focused on the reasons, consequences and control methods of the septicity and hydrogen sulphide production in sewer systems.

#### 5. Sludge treatment processes (M. Dřtil, M. Hutřian)

Laboratory and pilot scale research on autothermophilic aerobic sludge digestion and its comparison with other digestion methods (psychrophilic aerobic digestion, anaerobic digestion) was realised. Excess sludge from medium loaded activation at industrial WWTP was digested. Attention was given to sludge removal efficiency, quality of sludge water, dewatering properties and hygienisation of the sludge.

Sludge water treatment by sorption in alginite was tested. Main attention was given to ammonium and phosphates removal. In addition, effect of alginite on sludge sedimentation, thickening and dewatering was determined.

#### 6. Fenton and Photo-Fenton Reaction (J. Prousek)

Fenton reaction for the degradation of selected dyes such as Ostazine Yellow H-5G, Ostazine Blue H-P, Ostazine Green H-3G, and Brilliant Yellow have been studied. Similarly the Fenton reaction has been used for real coloured wastewater treatment with high initial COD and dye content values. Photo-Fenton and similar photochemical reactions have been tested for the degradation of dyes and some nitrogen heterocycles such as benzimidazole and its derivatives. Tested photochemical systems were as follows:  $\text{H}_2\text{O}_2/\text{Fe}^{2+}/\text{UV}$ ,  $\text{H}_2\text{O}_2/\text{Fe}^{3+}/\text{UV}$ ,  $\text{H}_2\text{O}_2/\text{Fe}(\text{C}_2\text{O}_4)_3^{3-}/\text{UV}$ ,  $\text{Fe}^{2+}/\text{H}_2\text{C}_2\text{O}_4/\text{UV}$ , and  $\text{Fe}^{3+}/\text{H}_2\text{C}_2\text{O}_4/\text{UV}$ . Best of all has been appeared the  $\text{H}_2\text{O}_2/\text{Fe}(\text{C}_2\text{O}_4)_3^{3-}/\text{UV}$  system.

#### 7. Study of the apoptosis effect of berberine on various cellular effects (M. Āřňáková)

Berberine is an isoquinoline derivative which was isolated from Mahonia aquifolium. It has long been known to have some antibacterial and antiprotozoal properties. Furthermore, it binds to DNA around the neutral pH by intercalation in the GC-rich regions of DNA. It has also been known that berberine has an ability to induce the apoptosis. In our work, the antimutagenic activity of berberine and the interactions of enzymes – topoisomerase (TOPO-I) and (TOPO II) with berberine were estimated. The *in vitro* cytotoxicity of berberine to human cancer cells of the line Hela and of murine leucemic cell lines L 1210 were investigated in relation to the cytotoxic activity of berberine and the action of its molecular mechanism. The toxicity of berberine to various cell models. The effect of berberine on various kinds of the plant and animal kingdom living in water. The observations were completed by a combined effect of the UV- and  $\gamma$ -radiation. The antimicrobial activity of berberine was estimated in the various kinds of clinical bacteria sensitive and resistant to antibiotics; yeasts and fungi.

### C. Penetration of Ionic Species across Skin, (Vasil Koprda)

In the case of body surface radionuclide contamination, the penetration of radionuclides across the human skin enhances internal contamination of an organism. To regulate this process, it is useful to decrease the penetration rate of radionuclides or to increase the skin penetration barriers. The main objective of the research was the kinetic study of the transport of radionuclides  $^{137}\text{Cs}$ ,  $^{60}\text{Co}$ ,  $^{90}\text{Sr}$ ,  $^{109}\text{Cd}$ ,  $^{147}\text{Pm}$  across the skin, to search for possibilities of reducing the transport of some compounds through skin, to enhance prevention of systemic body contamination by the formation of insoluble compounds and compounds with poor penetration qualities, by the formation of deposit in upper layers of skin, and using of absorption and retarding agents.

Two different types of animal permeation model of human skin: a) whole intact skin from abdominal region of 5-day rat (5DR), and b) whole intact skin from the same region of 9-day rat (9DR) were used to differentiate between transdermal and transfollicular permeation of radionuclide ions across the skin. To find out an existence of skin depot of permeated substances the skin splitted in epidermal-dermal junction was used. To define stratum corneum as the dominant permeation barrier the skin stripping was used.

The experimental results in diffusion chambers *in vitro* brought the following conclusions:

the 5DR skin was again found to be a suitable biological model for transdermal transport characterisation; the transport of metallic ions along hair follicles is important and in the case of the 9 DR skin it is even more pronounced than the transepidermal transport; the horny layer represents the most significant barrier to the penetration of ions; skin-protective and regenerative cream Indulona showed ion-permeation enhancing effect;

synthetic zeolite (zeolone) showed more suppressive features than natural zeolite (mordenite); the rate of ion penetration is proportional also to its amount in the donor solution, and reversely proportional to its charge; the ions were transported through skin in the decreasing order:  $\text{Cs}^+ > \text{Cd}^{2+} > \text{Sr}^{2+} > \text{Co}^{2+} > \text{Pm}^{3+}$ ; carboxymethyl-chitin-glucan was found the more efficient inhibitor of ion transport than fibrillar beta-glucan, and both showed concentration dependence of the inhibition; concentration of radionuclides in epidermis was found lower than in derma.

### D. Syntheses directed towards novel structurally well defined $\pi$ -conjugated heterocyclic compounds and their oligomers (Gabriel Āík)

The method of chemical oxidative polymerization with  $\text{FeCl}_3$  was used to synthesize the copolymer of dipyrido-[3,2-a; 2',3'-c]-thien-[3,4-c]azine and 3-dodecylthiophene. The copolymer was characterized by UV-VIS,  $^1\text{H}$  and  $^{13}\text{C}$  NMR and EPR spectroscopy. It has been found that copolymer exhibits properties of low-band-gap polymer. The formation of reactive oxygen species due to irradiation by visible light of thiophene oligomers incorporated in the pentasil-type Na-ZSM-5 zeolite microstructure has been studied in aqueous medium. The oxidative oligomerization of thiophene was carried out in the zeolite channels after ion exchange of  $\text{Na}^+$  for  $\text{Cu}^{2+}$ . By means of spin trapping, the hydroxyl radicals temporarily produced *in situ* were detected by EPR spectroscopy in aqueous suspension on the Cu-ZSM-5 sample with polythiophene deposited in the channels of the zeolite microstructure during illumination with visible light. Influence of the Cu(II)-complexes of thiophene oligomers synthesized by oxidative polymerization of thiophene with  $\text{Cu}^{2+}$  ions in ZSM-5 zeolite channels on fungicidal and antimicrobial properties was studied. It has been found that the heterogenous system culture medium-modified zeolite increases sporulation of the tested fungus (*Aspergillus niger*) and currently kills yeast (*Candida albicans*). As for the tested bacteria ( $G^+$  *Staphylococcus aureus*,  $G^-$  *Escherichia coli*), the percentage of the killed cells increases due to light activation of the system. The light effect is assigned to photogeneration of the reactive

oxygen species, mainly OH radicals, which were registered in the water solution by EPR spectroscopy.

## V. COOPERATION

### A. Cooperation in Slovakia

Amylum SLOVAKIA s.r.o., Boleráz,  
ASIO-SK s.r.o., Bytča

Association of Wastewater Treatment Experts in Slovak Republic,  
Bratislava

ČOVSPOL a.s. Bratislava

Department of Analytical Chemistry, Faculty of Pharmacy,  
Comenius University, Bratislava

Department of Nuclear Chemistry, Faculty of Natural Sciences,  
Comenius University, Bratislava

Department of Nuclear Physics, Faculty of Mathematic and Physics,  
Comenius University, Bratislava

Department of Physics, Faculty of Electrical Engineering and  
Information Technology, Slovak University of Technology, Bratislava

Department of Plant Physiology, Faculty of Natural Sciences,  
Comenius University, Bratislava

Ekologické služby, s.r.o. Strážske

Faculty of Pharmacy, Comenius University in Bratislava

Faculty of Natural Science, Department of Chemistry,  
Matej Bel University in Banská Bystrica

Institute of Chemistry, Faculty of Natural Sciences,

Comenius University, Bratislava

Institute of Experimental Pharmacology, Slovak Academy of Sciences,  
Bratislava

Institute for Education of Slovnaft Co., Bratislava

JANK GROUP a.s., Skalica

Kafiléria, a.s. Senec

Nuclear Regulatory Authority of the Slovak Republic, Bratislava

ROSLO s.r.o., Bratislava

Research Institute of Nuclear Power Stations, Trnava Ltd.

SANEK s.r.o., Bratislava

Severoslovenské celulózky a papierne, a.s. Ružomberok

Slovak Society for Industrial Chemistry of Slovnaft Co., Bratislava

Toxicological Section of Slovak Society for Industrial Chemistry,  
Bratislava

Toxicological Chemistry Section of SCS at Slovak Acad. of Sci.,  
Bratislava

Water Research Institute, Bratislava

(M. Hutňan, M. Drtil, M. Onderová, M. Horňák)  
(I. Bodík)

(I. Bodík, J. Derco, M. Drtil, A. Fargašová, E.  
Gašpariková, M. Horňák, M. Hutňan)  
(M. Drtil)

(M. Harangozó, A. Fargašová)

(P. Dillinger, M. Földesová, V. Koprda)

(P. Dillinger., M. Földesová, O. Holá)

(G. Čík)

(A. Fargašová)

(J. Derco)

(M. Čerňáková, V. Koprda)

(P. Dillinger., M. Földesová, M. Harangozó)

(G. Čík, A. Fargašová)

(V. Koprda, P. Bendová).

(V. Koprda)

(M. Hutňan, M. Onderová, M. Horňák)

(M. Hutňan)

(V. Koprda)

(V. Koprda, Z. Kassai, A. Palinkasová, P.  
Bendová)

(P. Dillinger., M. Földesová, V. Koprda)

(M. Hutňan, M. Onderová, M.

Horňák)

(J. Derco)

(V. Koprda)

(V. Koprda)

(V. Koprda)

(I. Bodík, J. Derco, P. Dillinger, M. Drtil, M.  
Földesová, M. Harangozó, M. Hutňan, V.  
Koprda)

### B. International Cooperation

ASIO s.r.o., Brno, Czech Republic,

- Waste water treatment processes (I. Bodík, M. Drtil)

Consiglio Nazionale delle Ricerche, Istituto di Chimica delle Macromolecole, Via E. Basini 15, 20133,

- Molecular materials and functional polymers (G. Čík)

Department of Chemistry and Physics, University of Agriculture, Cracow, Poland,

- Metal-metal interactions (A. Fargašová)

Faculty of Chemistry, VUT Brno, Brno, Czech Republic,

- Risk assessment of wood preservative compounds (A. Fargašová)

- Wastewater treatment technology (J. Derco)

School of Pharmacy, Dept. Pharm. Chem., King Edward VII. Ave, Cardiff, United Kingdom.

- Transcutaneous penetration of xenobiotics (V. Koprda).

Univ. Claude Bernard Lyon-1, ISPB, Dept. Galenic Pharm., Lyon, France.

- Transcutaneous penetration of xenobiotics (V. Koprda)

### C. Membership in Domestic Organizations and Societies

Association of Wastewater Treatment Experts in Slovak Republic,  
Bratislava

(I. Bodík, J. Derco, M. Drtil, A. Fargašová,  
M. Hutňan)

Biotechnological Society, Bratislava, Slovak Republic (M. Čerňáková)

Czechoslovak Limnological Society, Prague-Bratislava,

Czech Republic and Slovak Republic

(M. Čerňáková)

Czechoslovak Microbiological Society, Prague-Bratislava,  
Czech Republic and Slovak Republic  
Environmental Committee for Valuation and Identification of  
Products at the Ministry of the Environment SR  
Expert Group of State Office for Nuclear Safety  
Pharmacological Soc. of Slovak Medical Society, Bratislava  
Slovak Chemical Society, Bratislava

(M. Čerňáková)

(A. Fargašová)  
(V. Koprda)  
(V. Koprda)(G. Čík, J. Derco, P. Dillinger, A.  
Fargašová, M. Harangozó, V. Koprda, J.  
Prousek)

(V. Koprda)

(A. Fargašová, M. Harangozó, V. Koprda)  
(J. Derco, M. Hutňan)(I. Bodík, J. Derco, M. Drtil, P. Dillinger, A.  
Fargašová, M. Földesová, M. Hutňan)

(M. Čerňáková, A. Fargašová)

(V. Koprda)

Slovak Nuclear Society, Bratislava  
Slovak Pharmaceutical Society at SMS Bratislava  
Slovak Society of Chemical Engineering, Bratislava  
Slovak Society of Industrial Chemistry, ZSVTS, Bratislava

Slovak Society of Limnology at SAS Bratislava  
Society of Nuclear Medicine and Radiation Hygiene of SMS, Bratislava

**D. Membership in International Organizations and Societies**

Association of Wastewater Treatment Experts, Brno, Czech Republic

(I. Bodík, J. Derco, M. Drtil, A. Fargašová, E.  
Gašpariková, M. Hutňan, M. Horňák)

Bulletin of Environmental Contamination and Toxicology,  
U.S.A. – Member of Editorial Board  
Czech Chemical Society, Prague, Czech Republic  
International Water Association, London, UK  
European Photochemistry Association, Mülheim, Germany  
EUROTOX Madrid, Spain  
FECS Division on Chemistry and the Environment  
Journal of Trace and Microprobe Techniques,  
U.S.A. – Member of International Group of Correspondents  
SECOTOX – International Society of Ecotoxicology and  
Environmental Safety, Munich, Germany

(A. Fargašová)

(V. Koprda, J. Prousek)

(I. Bodík, J. Derco)

(G. Čík, J. Prousek)

(A. Fargašová)

(V. Koprda)

(A. Fargašová)

(A. Fargašová)

**E. TEMPUS Programme**

TEMPUS JEP-IB 13123/98

Coordinator: Anežka Moncmanová

Coordinating institution: STU, Bratislava

Title: Continuing Education in European Directives and Environmental Standards

Partners:

Universita degli Studi, Bari, Italy, TEMPUS Project

Vienna University of Technology, Vienna, Austria, TEMPUS Project

Institut für Ökologie, St. Pölten, Austria, TEMPUS Project

NOWATECH, Ass., Bari, Italy, TEMPUS Project

ENEA, Rome, Italy, TEMPUS Project

Zväz hutníctva, ťažobného priemyslu a geológie SR, Bratislava

ASIO s.r.o., Bytča

Technická univerzita Zvolen, Fakulta ekológie a environmentalistiky, Zvolen

Duration: December 1998 to March 2001

**F. International Scientific Programmes**

COST Action 837 „Plant biotechnology for the removal of organic pollutants and toxic metals from wastewaters and contaminated sites“ (A. Fargašová)

Working Group 2 (WG2) – Toxic metals: screening and uptake studies

Working Group 4 (WG4) – Cultivation and utilization of plants

Coordinator: Dr. J. P. Schwitzguebel, Lausanne, Switzerland

Coordinators for Slovak Republic: Assoc Prof. A. Lux, Faculty of Natural Science, Comenius University, Bratislava; RNDr. D. Lišková, PhD., Institute of Chemistry SAS, Bratislava Partners: On the project participate 21 countries (the list of participants can be found on <http://lbewww.epfl.ch/COST837>)

Period: April 1998 to April 2002

**G. Visitors from Abroad**

Prof. M. Dohanyos

Prof. J. Wanner

VŠCHT Praha, Czech Republic, January 2001 (1 day)

VŠCHT Praha, Czech Republic, April 2001, October 2001, November 2001 (5 days)

ASIO Brno, Czech Republic, November 2001 (2 day)

LU Vienna, Austria, November 2001 (2 days)

TU Budapest, Hungary, November 2001 (1day)

FSU, Jena, Germany, May 2001 (3 days)

GSF-Nat.Res.Center for Environ. and Health, Neuherberg, Germany, June 2000 (1 day)

Chem.Faculty UT Brno, Czech Rep., April 2001 (1 day)

Ing. K. Plotěný

Dr. Ing. T. Ertl

Assoc. Prof. D. Dulovics

Prof. M. Anke

Dr. K.-W. Schramm

Prof. J. Matoušek

**H. Visits of Staff Members and Postgraduate Students in Foreign Institutions**

|                |   |
|----------------|---|
| Bodík I.       | Vienna University of Technology, Austria, January 2001 (2 days)   |
| Bodík I.       | Universita degli Study Bari, Italy, February 2001 (5 days)  |
| Bodík I.       | Conference "Anaerobic Treatment 2001", Klatovy, Czech Republic, October 2001 (3 days)   |
| Bodík I.       | Seminar "Legislative für die Kleinkläranlagen im Mitteleuropa", Kobilí (Czech Republic) January 2001, (2 days)                  |
| Drtíl M.       | Association of Wastewater Treatment Experts, Prague, Brno, Czech Republic, March, June, September 2001, (6 days)                |
| Gašparíková E. | EuroLab Course "Pollution Surveillance and Control in Wetland Ecosystems, University of Veszprém Hungary, October 2001 (6 days) |
| Hornák M.      | International Conference "Water and Environment", Pavlov, Czech Republic, November 2001 (2 days)                                |
| Hutňan M.      | Prague Institute of Chemical Technology, Prague, Czech Republic, June 2001 (1 day)  |
| Hutňan M.      | Association of Watertreatment Experts of Czech Republic, Brno, Czech Republic, September 2001 (2 days)                          |
| Hutňan M.      | Conference "Anaerobic Treatment 2001", Klatovy, Czech Republic, October 2001 (3 days)   |
| Hutňan M.      | Vienna University of Technology, Austria, January 2001 (2 days)   |
| Moncmanová A.  | Vienna University of Technology, Austria, January 2001 (2 days)   |

**VI. THESES AND DISSERTATIONS****A. Graduate Theses (MS Degree) for state examinations after five years of study (supervisors are written in brackets):**

|                  |   |
|------------------|---|
| Adamčík M.:      | The study of sorption conditions of Sn with natural sorbents by method of radiotracer. (P.Dillinger)  |
| Angušová L.:     | Anaerobic treatment of sugar beet pulp. (M. Hutňan)   |
| Bartošová N.:    | Ecotoxicological effects of copper complexes on freshwater algae. (A. Fargašová)  |
| Bendová Petra:   | The study of permeation of substances across the skin animal models. (V.Koprda)   |
| Gašparíková E.:  | The influence of the temperature on the anaerobic degradation of the primary sludge. (I. Bodík)   |
| Godóová E.:      | The study of the sorption of Sn and competitive cations Fe, Co, Cs by radioexchange and AAS methods. (M. Földesová)   |
| Hájnik P.:       | The use of radioexchange method for the studying of sorption and desorption of Sn by various types of zeolites. (P. Dillinger)  |
| Jankuliaková M.: | The use of radioexchange and AAS methods for the studying of sorption and desorption Sn and competitive ions Cr, Zn, Cu by natural and chemically modified zeolites. (M. Földesová) |
| Kočanová S.:     | Comparison of psychrophilic and thermophilic aerobic sludge digestion. (M. Drtíl)   |
| Kuruc M.:        | Utilisation of ozone for transformation of biologically resistant organics. (J. Derco)  |
| Okruhlicová T.:  | Incineration of solid wastes in Duslo Šafa a.s. (M.Harangozó)   |
| Pajgerová L.:    | Utilisation of auto-thermophilic aerobic sludge digestion at industrial WWTP. (M. Drtíl)  |
| Plodová M.:      | The programmed death of cell-apoptosis induces by berberine isolated from Mahonia. (M. Čerňáková)   |
| Tamášiová L.:    | The content of heavy metals in wheat in dependencene on the soil composition. (M.Harangozó)   |
| Vavreková L.:    | Degradation of selected water pollutants by Fenton- and modified Fenton reaction. (J. Prousek)  |
| Žemberová M.:    | Photodegradation of selected environmental pollutants by the use of photocatalysis and photo-Fenton reaction. (J. Prousek)  |

**B. Dissertations (PhD)**

|                |   |
|----------------|---|
| Buday J.:      | Intensification of nitrogen removal from wastewater – substrate and product inhibition of nitrification. (Derco, Drtíl)   |
| Kassai Z.:     | Effect of patterns of chemical substances on their transdermal permeation and possibility to influence the permeation by chemical substances. (Koprda, Harangozó) |
| Kovács A.:     | Modelling of biological processes of nutrient removal. (Derco)  |
| Miháliková E.: | Monitoring of chemical characteristics of size fractions of air aerosols regarding evaluation of their potential health risk. (Koprda)                            |
| Mrafková L.:   | Anaerobic treatment of wastewater in high rate reactors. (Derco, Hutňan)  |

**C. Dissertations (DrSc.)**

Fargašová A.: Ecotoxicological tests utilization for metal toxicity determination on selected environmental components. FEE TU Zvolen.

**D. Habilitation Theses**

Brokeš P.: Possibilities of the use of membrane processes for recycling of wastewater and secondary raw materials, Field: Chemistry and technology of environment, Sci. branch 28-95-9

Drtíl M.: Selected problems of kinetics and regulation of processes of biologic removal of nitrogen, Field: Chemistry and technology of environment, Sci. branch 28-95-9

Krištín J.: Characteristics of aerosols in outdoor air, Field: Chemistry and technology of environment, Sci. branch 28-95-9

**VII. PUBLICATIONS****Journals (\*registered in Current Contents)**

- [1]\* Bauerová K., Kassai Z., Koprda V., Harangozó M: Contribution to the penetration of radionuclides across the skin. Concentration dependence of strontium through the skin In Vitro. J. Appl. Toxicol. 21, 241-243 (2001)
- [2] Bodík I.: Voda v internete, internet vo vode. Water in internet, internet in water (in Slovak). XXI. storočie 4(3), 55-56 (2001).
- [3] Bodík I., Rajczyková E.: Základné problémy súčasného odvádzania a čistenia odpadových vôd v SR. The basic problems of the present draining and treatment of wastewater in the Slovak Republic (in Slovak). XXI. storočie 4(1), 30-32 (2001).
- [4]\* Čík G., Krajčovič J., Veis P., Végh D., Šeršeň F.: Characterization and properties of the copolymer of dipyrido-[3,2-a; 2,3-c]-thien-[3,4-c]azine with 3-dodecylthiophene. Synth. Met. 118, 111-119 (2001)
- [5]\* Čík G., Šeršeň F., Bumbálová A.: In situ spin trapping of OH radicals photochemically generated by thiophene oligomers incorporated in copper-doped ZSM-5 zeolite in aqueous medium. Microporous and Mesoporous Materials 46, 81-86 (2001)
- [6]\* Čík G., Bujdaková H., Šeršeň F.: Study of fungicidal effect of the Cu(II)-complexes of thiophene oligomers synthesized in ZSM-5 zeolite channels. Chemosphere 44, 313-319 (2001)
- [7]\* Čík G., Šeršeň F., Dlháň L.: Electric conductivity of poly(3-dodecylthiophene) and its dependence on the conformational changes of polymer chains. Czech. J. Phys. 51, 257-271 (2001)
- [8] Derco J., Kuffa R., Marová J.: Vplyv zrážacích činidiel na sedimentačné a odvodňovacie vlastnosti kalu. Influence of precipitation agents on sedimentation and dewatering properties of activated sludge. (In Slovak). Vodní hospodářství, 5 (2001). Čistírenské listy 3, XI - XII (2001).
- [9] Derco J., Kuffa R., Marová J.: Vplyv zrážacích činidiel na sedimentačné a odvodňovacie vlastnosti kalu. Influence of precipitation agents on sedimentation and dewatering properties of activated sludge. (In Slovak). Vodní hospodářství, 7 (2001). Čistírenské listy 4, V -VII (2001).
- [10] Derco J.: Procesy prebiehajúce v stokovej sieti. Processes in sewer system (In Slovak). Vodohospodársky spravodajca, 44 (1), 13 - 14, (2001).
- [11] Derco J., Kovács A. Odstraňovanie nutričov v aktivácii s časovou segregáciou. Nutrient removal in an intermittently aerated activated sludge process (in Slovak). Vodohospodársky spravodajca, 11, 8 - 10, (2001).
- [12]\* Derco J., Králik M., Kovács A.: Modelling of Nutrient Removal Processes in an Intermittently Aerated Bioreactor. Chem. Biochem. Eng. Q. 15 (4), 167 - 174, (2001).
- [13] Derco J. Intenzifikácia procesov čistenia odpadových vôd znečistených ropnými a olejovými látkami. Intensification of an oil wastewater treatment processes (In Slovak). Ropa a uhlie 43 (1), 39 - 41, (2001).
- [14] Derco J., Gulyášová A., Králik M., Mrafková L.: Treatment of an industrial wastewater by ozonation. Petroleum and Coal 43 (2) 92-97 (2001).
- [15] Derco J., Králik M.: Optimisation of an oil wastewater treatment plant. Petroleum and Coal 43 (2) 85-88 (2001).
- [16] Drtíl M., Bodík I., Belica P.: Základné problémy súčasného odvádzania a čistenia komunálnych odpadových vôd. Actual problems of municipal wastewater collection and treatment (in Slovak). Eurostav 7/ 6, 10-12 (2001)
- [17]\* Fargašová, A.: Winter fourth instar larvae of *Chironomus plumosus* as bioassay tools for assessment of acute toxicity of metals and their binary combinations. Ecotoxicol. Environ. Saf. 48, 1-5 (2001)
- [18]\* Fargašová, A.: Effect of Cd in combination with Cu, Zn, Pb and Fe on root elongation and metal accumulation in the roots and cotyledones of mustard (*Sinapis alba*) seedlings. Rostl. Vyr. 47(3), 97-103 (2001)
- [19]\* Fargašová, A.: Phytotoxic effects of Cd, Zn, Pb, Cu and Fe on *Sinapis alba* L. seedlings and their accumulation in roots and shoots. Biol. Plantarum 44(3), 471-473 (2001)
- [20]\* Fargašová, A.: Interactive effect of manganese, molybdenum, nickel, copper I and II, and vanadium on the freshwater alga *Scenedesmus quadricauda*. Bull. Environ. Contam. Toxicol. 67, 688-695 (2001)
- [21] Fargašová, A., Ondrejkočiová, I., Havránek, E., Štofeková, O.: Environmental risk assessment of Cd(II) complexes with N-donor ligand nicotinamide to freshwater phytoplankton. In: Melník, M., Sirota, A. (Eds.): Challenges for Coordination Chemistry in the New Century, Vol. 5., Slovak Technical University Press, Bratislava 2001, p. 265-270, (2001) ISBN 80-227-1539-5, ISSN 1335 - 308X
- [22] Gejdoš M., Derco J.: SČOV Ružomberok - prevádzkové skúsenosti s čistením odpadových vôd. SČOV Ružomberok - operational experience with wastewater treatment (In Slovak). Vodohospodársky spravodajca, 12, 18 - 20, (2001).
- [23]\* Habuštová O., Weismann L., Harangozó M., Bumbálová A.: Determination of copper in pupae and adults of the Colorado potato beetle (*Leptinotarsa decemlineata* Say) by radionuclide X-ray fluorescence technique. J. Radioanal. Nucl. Chem. 247, 575-576 (2001)
- [24]\* Hutňan M., Drtíl M., Mrafková L.: Anaerobic biodegradation of sugar beet pulp. Biodegradation 11, 203-211 (2000)
- [25]\* Hutňan M., Drtíl M., Derco J., Mrafková L., Horňák M., Mičo S.: Two-step pilot-scale anaerobic treatment of sugar beet pulp. Polish J. Env. Stud. 10, 237-243 (2001)
- [26]\* Hutňan M., Horňák M., Drtíl M.: Využitie vysladených rečných rezkov na výrobu bioplynu. III. Opätovný nábeh procesu a

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- [10] Tölgyessy J., Harangozó M., Daxnerová O: Monitoring životného prostredia. Environmental Monitoring (in Slovak). FPV UMB, Banská Bystrica, 175 pp. (2001)

## DEPARTMENT OF FIBRES AND TEXTILE CHEMISTRY

### Head of the Department:

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### I. STAFF

#### Full Professor:

Eberhard Borsig, PhD, DSc

#### Associate Professors:

Pavol Hodul, PhD, Michal Krištofič, PhD, Anton Marcinčin, PhD

#### Assistant Professors:

Jaroslav Legéň, PhD, Anna Ujhelyiová, PhD

#### Research Fellows:

Eva Bolhová, Marcela Hricová, Anna Murárová, PhD, Elena Zemanová, PhD

#### PhD Students:

Natália Karabcová, Eva Körmendyová, Zita Mlynarčíková, Silvia Pavlíková

#### Technical Staff:

Daniela Dančová, Gabriel Kužel, Albína Pokorná, Edita Štábelová

### II. TEACHING AND RESEARCH LABORATORIES

#### A. Teaching Laboratories:

Laboratory of Macromolecular Chemistry

Laboratory for Computer Modeling of Structure and Properties of Polymers

Laboratory of Polymer Fibre and Fibrous Material Structure (DSC, TMA, SALS, Surface Properties)

Laboratory of Fibre Technology

Laboratory of Textile Chemistry, Bleaching, Dyeing and Finishing

Laboratory of Fibre and Textile Testing

Laboratory for fibre spinning, drawing and texturing, extruders 16 and 30 mm

Laboratory for dyeing and finishing of fibres and textile materials (Ahiba, Pretema, Multicolor)

#### B. Research Laboratories:

Equipments:

DSC-Perkin Elmer and DTA (Derivatograph Q 1500 D)

TMA-50 M and TA (thermomechanical measurement)

Instron, model 1112 and Uster for mechanical properties

Dynamic viscoelastomer model Rheo-200

Alambeta for measurement of thermo - properties of textiles

Integral electrometer Polystat PS-1

Capillary rheometer

Computers PC-AT and XT

Unimode semiconductive laser 25mW, 690nm with universal optical set

Microscope Olympus model BHT

Laboratory equipments for light degradation of fibrous materials-Xenotest

for exhaust dyeing process and its evaluation ((Ahiba, Pretema, Multicolor)

Spinning machines with extruders,  $\varnothing$  16 mm and 30 mm respectively

### III. TEACHING

#### A. Undergraduate Study

##### 5th Semester (autumn)

|                          |         |        |
|--------------------------|---------|--------|
| Macromolecular Chemistry | (2-0 h) | Borsig |
|--------------------------|---------|--------|

##### 6th Semester (spring)

|                               |           |           |
|-------------------------------|-----------|-----------|
| Technology of Materials       | (2-0 h)   | Marcinčin |
| Cosmetic and Indoor Chemistry | (2-0 h)   | Hodul     |
| Bachelor Project              | (0-0-4 h) |           |

##### 7th Semester (autumn)

a) compulsory subjects:

|                               |         |                  |
|-------------------------------|---------|------------------|
| Macromolecular Chemistry II   | (2-1 h) | Borsig           |
| Physics of Polymers and Paper | (2-2 h) | Krištofič        |
| Fiber Sci. and Technology     | (2-2 h) | Marcinčin, Legéň |

|   |           |                             |
|---|-----------|-----------------------------|
| Laboratory of Fiber Sci. and Technology       | (0-0-8 h) | Krištofič, Legéň, Karabcová |
| b) optional subjects:                         |           |                             |
| Structure of Fibrous Materials                | (1-1 h)   | Ujhelyiová, Murárová        |
| Modelling of Polymer Structure and Properties | (1-1 h)   | Rychlý, Marcinčin           |

**8th Semester (spring)**

|  |           |                            |
|--|-----------|----------------------------|
| a) compulsory subjects:                |           |                            |
| Colorants and Textile Auxiliaries      | (2-0 h)   | Hodul, Murárová            |
| Technical Textiles                     | (2-0 h)   | Krištofič, Borsig          |
| Principles of Textile Engineering      | (2-0 h)   | Ujhelyiová, Murárová       |
| Laboratory of Textile Engineering      | (0-0-8 h) | Legéň, Hodul, Mlynarčíková |
| b) optional subject:                   |           |                            |
| Physiology and Comfort of Clothing     | (0-2 h)   | Murárová                   |
| Special Chemical Treatment of Textiles | (0-2 h)   | Ujhelyiová, Murárová       |

**9th Semester (autumn)**

|  |            |                           |
|--|------------|---------------------------|
| Textile Chemistry and Technology               | (2-2 h)    | Hodul, Murárová           |
| Technology of Polym. Films                     | (2-0 h)    | Marcinčin, Ujhelyiová     |
| Laboratory of Textile Chemistry and Technology | (0-0-10 h) | Hodul, Pavlíková, Bolhová |
| Fiber and Textile Testing                      | (2-0 h)    | Legéň, Ujhelyiová         |

**10th Semester (spring)**

|                |            |
|----------------|------------|
| Seminary       | (0-3-0 h)  |
| Diploma Thesis | (0-0-27 h) |

**B. PhD study:**

|                                   |           |
|-----------------------------------|-----------|
| a) subjects:                      |           |
| Physics of Polymers               | Krištofič |
| Macromolecular Chemistry          | Borsig    |
| Technology of Polymeric Materials | Marcinčin |
| Organic Chemistry                 |           |
| Physical Chemistry                |           |

## b) Seminars

Experience from international conferences on polymers held in the year 2000, E.Borsig, Jan. 12, 2001  
 Polypropylene composite fibres, S. Pavlíková, Jan. 21, 2001  
 Modification of polymers by solid additives A. Marcinčin, Feb. 8, 2001  
 Isotopically pure uniform polymers, O. Vogl, March 2<sup>nd</sup>, 2001  
 Evaluation of fibres by TMA method, E. Zemanová, March 16, 2001  
 Technical fibres and textiles, Š. Kišš, Tatrabant, May 14, 2001  
 Mechanical and thermal properties of PP/PA blend, Z. Mlynarčíková, Dec. 7, 2001

**IV. CURRENT RESEARCH PROJECTS****A. Dispersion of organic pigments in synthetic polymers with particle size close to nano-scale (Anton Marcinčin)**

The aim of the project is a solution of miscibility of polypropylene PP with polar polymers (PA, PET) and also with other additives with respect to achieve a spinning of these blends. A polymer blend consisting of PP, branched PE and PET was studied by the DSC method. If PE was present in the blend in a minority amount an increase of amorphous phase and on the contrary an increase of crystallinity position in PP component were observed. The results showed that a partial miscibility of PP and LDPE over melting point was observed. On the other hand an decrease of PET crystallinity portion, which forms a disperse phase, was observed it is proportional to its amount in the blend. These morphological changes influence the sorption of dispersion dyes of the blend fibers.

Investigations of pigment dispersability in polypropylene (PP) and polyethylene terephthalate (PET), evaluation of the polymeric additives influence and processability of the system PET + pigment Black 7 during the preparation of fibres were examined.

On the base of the rheological measurements and mechanical-physical properties of fibres some low molecular additives for dispergation of antibacterial additives in PP fibres and the composition of blended fibres PET-polybutyleneterephthalate-Black 7 (with better dispergation of Black 7) were found.

**B. Fibre-forming Polypropylene-Polar Polymer Blends (Eberhard Borsig)**

In the framework of this project polypropylene fibres modified with polymer additives based on:

a) polyethylene terephthalate

b) etylen - vinylacetate copolymer (EVAC)

and with some low- and high-molecular compatibilizers e.g. reactive compatibilizer - PP grafted by maleinanhidrid (PP-MAH) and alkyldiamid of carboxylic acid (ADCA) were prepared and their properties were investigated as well.

Influence of these compatibilizers on morphology of blend PP/PET fibres was investigated. Favourable influence of ADCA on compatibility of PP and PET components was found and this system rends multifibrillar type of fibres with higher elastic properties and higher sorption of disperse dyes as well. By using polyvinylacetate and ethylene-vinylalcohol copolymer this polyfibrillar structure of fibres becomes finer or even get lost. Simultaneously a good processability and disperse dyes uptake is conserved.

Some experiments about the preparation of PP composite fibres, using the filter SO MASIF C16 (capable to create inorganic nano-partides) and PP-MAH as the compatibiliser were made as well. Composite PP fibres were drawn at different drawing ratios which influence the degree of exfoliation and that of crystallization of created nano-particle as well. Nano-particle in PP fibres

generally cause a decrease the fibre tensile strength but elongation (orientation) of fibres cause a relatively higher increase of their tensile strength than at non-filled PP fibres. In some cases the tensile strenght of oriented fibres is very close to that of non -filled PP fibres with the same drawing ratio.

Thermal characteristics of blended PP/PET fibres (melting temperature,  $T_m$ , enthalpy of fusion,  $\Delta H_m$ , at first and second heating, enthalpy of crystallization,  $\Delta H_c$ ) were estimated and showed (besides the supposed thermodynamical incompatibility) mutual influence of two components of polymer blend. Minor component accelerates crystallization ability of major component. Non-isothermal measurements of these fibres led to the calculation of surface energi of crystallites in PP/PET fibres.

The results of thermo-mechanical measurements showed that higher elasticity and relaxation of PP/PET fibres is a consequence of the absence of interphase compound.

Modified PP fibres have better dyeability by exhaustion process. Dye uptake from the dyeing bath is considerably influenced by modification of fibre in the lateral and longitudinal direction. Changes in the linear density and mainly in the shape of fibre cross-section essentially improve dyeability of fibres which can be evaluated by K/S value from Kubelka-Munk equation.

PP/PET fibres with triangular 3 hollow cross-section have K/S value nearly 5 times higher in comparison with classic circular cross-section.

PP/EVAC blend circular fibres have their K/S value 4-13 times higher according to the amount and type of EVAC (5wt.% - 15wt.%) and according to the presence or absence of ADCA agent. Some other properties of yarns formed from these modified PP fibres (mainly physiologic) can be improved.

## V. COOPERATION

### A. Cooperation in Slovakia

Research Institute for Man-Made Fibres, Svit  
 Research Institute of Textile Chemistry, Žilina  
 Polymer Institute, Slovak Academy of Sciences, Bratislava  
 Slovenský hodváb a.s., Senica  
 Chemosvit a.s., Svit  
 Rhodia Industrial Yarn a.s., Humenné  
 Nylstar a.s., Humenné  
 Merina a.s., Trenčín  
 Istrochem a.s., Bratislava

### B. International Cooperation

Chemical Fibre Institute, Lodž, Poland  
 - Organisation of the 2<sup>nd</sup> Central European Conference  
 Technical University, Liberec, Czech Republic  
 - Exchange of staff members and students in the CEEPUS network  
 University of Maribor, Faculty of Mechanical Engineering, Maribor, Slovenia  
 - Cooperation in the CEEPUS project  
 University of Zagreb, Faculty of Textile Technology, Croatia  
 - Cooperation in the CEEPUS project

### C. Membership in Domestic Organizations and Societies

|   |  |
|---|--|
| Advisory Board of scientific Journal Autex Res. J.                                      | (A. Marcinčin)   |
| Chairman of Editorial Board of scientific journal Vlákna a textil (Fibres and Textiles) | (A. Marcinčin)   |
| Advisory Board of scientific journal Vlákna a textil (Fibres and Textiles),             | (A. Marcinčin, P. Hodul, A. Ujhelyiová, A. Murárová)                                   |
| Executive Editor of scientific journal Vlákna a textil (Fibres and Textiles),           | (P. Hodul)   |
| Co-editor of scientific journal Vlákna a textil (Fibres and Textiles),                  | (A. Ujhelyiová, A. Murárová)   |
| Commission of the Grant Agency VEGA of the Ministry of Education and Science SR         | (A. Marcinčin)   |
| Slovak Chemical Society, Bratislava   | (E. Borsig, P. Hodul, M. Krištofič, A. Murárová, J. Legéň, E. Zemanová, A. Ujhelyiová) |

### D. Membership in International Organizations and Societies

|  |                |
|--|----------------|
| Association of Universities for Textiles (AUTEX), Gent, Belgium                                | (A. Marcinčin) |
| Committee for Slovak-Polish Conference   | (A. Marcinčin) |
| Scientific council TU Liberec, Czech Rep.  | (A. Marcinčin) |
| EPF, European Polymer Federation, Eindhoven, Holland   | (E. Borsig)    |
| Scientific Committe of Polymer Congres EPF   | (E. Borsig)    |
| Advisory Board of Scientific Journal Chemické listy (Chemical Letters), Prague, Czech Republic | (E. Borsig)    |
| Journal of Macromolecular Science, Pure and Applied Chemistry, USA,                            | (E. Borsig)    |

### E. Tempus Programme

### F. International Scientific Programmes

CEEPUS  
 SI-007 Objective Measurements Technology in Textile and Clothing Engineering  
 M. Krištofič, network is formed by:  
 Faculty of Mechanical Engineering, University of Maribor, Slovenia - coordinator

Faculty of Textile Technology, University of Zagreb, Croatia  
 Faculty of Textile Science Technical University of Liberec, Czech Republic  
 Textile Faculty, Technical University of Łódź, Poland  
 Faculty of Mechanical Engineering, Technical University of Budapest, Hungary  
 Faculty of Mechanical Engineering, Technical College for Light Industry, Hungary  
 January - December 2001

### G. Visitors from Abroad

|                          |  |
|--------------------------|--|
| Nagy Veronika            | Budapest University of Technology and Economics (BUTE) Hungary, January 10 - February 8 (CEEPUS) |
| Studničková Jarmila      | Technical University of Liberec, Czech Rep. April 26 - May 24 (CEEPUS)                           |
| Martincová Alice         | Technical University of Liberec, Czech Rep. March, 1 <sup>st</sup> - 30 (CEEPUS)                 |
| Dr. Kokas-Palicska Livia | Technical College for Light Industry, Budapest, Hungary, May 25-June 4, (CEEPUS)                 |
| Feher Csilla             | Technical College for Light Industry, Budapest, Hungary, June 18-July 13, (CEEPUS)               |
| Wilk Eva                 | Technical University of Łódź, Poland, June 19-July 13, (CEEPUS)                                  |

### H. Visits of Staff Members and PhD Students to Foreign Institutions

|                 |   |
|-----------------|---|
| E. Borsig       | EPF Symposium Eidhoven, July 2001, (The Netherlands), 3 days  |
| E. Borsig       | Swiezedov Zdroj, September 2001, (Poland), 2 days   |
| E. Borsig       | Albert-Ludwigs Universität Freiburg, May 2001, (Germany), 30days  |
| S. Pavlíková    | University Gent, ERASMUS-SOCRATES, July 3.-Sept. 30, 2001, (Belgium), 30 days   |
| Z. Mlynářčiková | University Gent, ERASMUS-SOCRATES, July 3.-Sept. 30, 2001, (Belgium), 30 days   |
| A. Marcinčin    | University of Terasse (Spain), University do Miřho (Portugal), Tecnitex 2001 (Technical Textiles), and 2001 International Textile Congres, June 16- July 3, 2001, 19 days |

Visits of Students to Foreign Institutions:

|                |  |
|----------------|--|
| Barníková, A.  | TU Liberec, Czech Rep. (CEEPUS), March-April 2001, 1 month                                 |
| Karabcová, N.  | Technical College for Light Industry Budapest, Hungary (CEEPUS), March-April 2001, 1 month |
| Chovancová, L. | BUTE, Hungary (CEEPUS), March-April 2001, 1 month  |
| Križanová, Z.  | TU Liberec, Czech Rep. (CEEPUS), March-April 2001, 1 month                                 |

## VI. THESES AND DISSERTATIONS

### A. Graduate Theses (MS Degree) for state examinations after five years of study (supervisors are written in brackets)

- Barníková A.: Influence of rheological properties of pigmented concentrates on spun-dyeing process of synthetic fibres (Marcinčin A.)
- Bernáth J.: Decolourization of waste water after dyeing with reactive dyes (Hodul P.)
- Bolhová E.: Thermal properties of blended synthetic fibres (Ujhelyiová, A.)
- Chovancová L.: Preparation of polypropylene composite fibres filled with inorganic filler (Borsig E.)
- Karabcová N.: Synthetic fibres based on polymer blend with modified cross-section (Legéň J.)
- Kolníková E.: Evaluation of supermolecular orientation of synthetic fibres (Zemanová E.)
- Križanová Z.: Evaluation of geometric and structural unevenness of synthetic fibres (Ujhelyiová A.)
- Kucháriková D.: Physical modification of synthetic fibres for improving some properties (Kriřtovič M.)
- Rafajová A.: Influence of geometric parameters of PET fibres on their dyeing (Murárová A.)

### B. Dissertations (PhD)

### C. Dissertations (DSc)

### D. Habilitation Thesis

## VII. PUBLICATIONS

### A. Journals (\*registered in Current Contents)

- [1]\* Kósa, Cs., Danko, M., Fiedlerová, A., Hrdlovič, P., Borsig, E., Weiss, R. G.: Pyrenyl Fluorescence as a Probe of Polymer Structure and Diffusion in a Polyethylene: Poly(butylmetacrylate)-co-polystyrene Interpenetrating Network and Related Polymers. *Macromolecules* 34, 2673-2681 (2001)
- [2]\* Greco, R., Iavarone, M., Fiedlerová, A., Borsig, E.: Optical properties of IPN-like networks

- polyethylene/poly(butylmethacrylate-co-styrene) copolymer systems. III. Influence of copolymer crosslinker. *Polymer* 42, 5089-5095 (2001)
- [3]\* Danko, M., Hrdlovič, P., Borsig, E.: Spectral Characteristics of Free and Linked Pyrene-Type Chromophores in Solution, Polymer Matrices, and Interpenetrating Networks. *J. Macromol. Sci.-Pure Appl. Chem.* A38(5&6) 467-486 (2001)
- [4]\* Borsig, E., Thomann, R., Fiedlerová, A., Müllhaupt, R.: Morphology of the Transparent IPN-like System PE: (BMA-co-S). *J. Appl. Polym. Sci.*, 81, 2615-2620 (2001)
- [5]\* Marcinčin, A., Jurčišinová, Z., Borsig, E., Krištofič, M., Marcinčinová, T.: Fiber - forming Blend Polypropylene-Polyvinyl Alkohol. *Polym. Adv. Technol.* 12, 461-465 (2001)
- [6]\* Borsig, E., Fiedlerová, A.: Transparentný systém vzájomne preniknutých polymérových sietí. Transparent System of an Interpenetrating Polymer Networks. *Plasty a kaučuk, Plastics and Rubber* 38, 70-73 (2001)
- [7] Hodul, P., Korcová, D., Lokaj, J., Murárová, A.: Effect of Additives on Soil Removal in Crease Resistant Finishing. *Vlákná a textil* 8(1) 8-12 (2001)
- [8] Murárová, A.: Fyziológia odievania I. Tepelná regulácia človeka. Physiology of Clothing I. Men's Thermal Regulation. *Vlákná a textil* 8(1) 48-49 (2001)
- [9] Murárová, A.: Fyziológia odievania II. Odev ako "fyziologický" systém. Physiology of Clothing II. Apparel as a Physiological System. *Vlákná a textil* 8 (1) 50-52 (2001)
- [10] Jambrič, M., Budzák, D., Marcinčin, A., Revús, M.: História rozvoja chemických vlákien vo svete a na Slovensku. Current Development of Chemical Fibers-Wide and in Slovakia. *Vlákná a textil* 8 (2) 77-89 (2001)
- [11] Marcinčin, A.: Synthetic Fibres Based on Polymer Blends. *Vlákná a textil* 8 (2) 126-134 (2001)
- [12] Hodul, P.: Biotechnológie v textilnom zošľachtovaní. Biotechnology in Textile Finishing. *Vlákná a textil* 8 (3) 211-217 (2001)
- [13] Smole, S. M., Zemanová, E.: Structure and Properties of Supercritical Fluid, Water and Hot Air Treated PET Fibres. *Vlákná a textil* 8 (2) 184-186 (2001)
- [14] Marcinčin, A., Brejka, O., Budzák, D., Hricová, M.: Vývoj polypropylénových vlákien farbiteľných vyťahovacím postupom a potlačou. Development of polypropylene fibres dyeable by exhaust proces and printing. *Vlákná a textil (Fibres and Textiles)* 8(1), 2001, p. 36-41
- [15] Marcinčin, A., Ujhelyiová, A.: Pigmentácia syntetických vlákien v hmote. Masspigmenting of Synthetic Fibres. *Vlákná a textil*, 8(1), 2001, p. 42-47

## B. Conferences (\*international conferences)

- [1]\* Borsig, E., Lazár, M., Fiedlerová, A., Hrkčková, L., Marcinčin, A.: Some aspects of the solid state polypropylene grafting using peroxides. In: CD-ROM Proceedings of the European polymer Federation (EPF) Congress, Eindhoven (The Netherlands), July 15 - 20, 2001, Session 3, KN9
- [2]\* Murárová, A., Hodul, P., Jambrič, M.: Influence of Geometric PET Fibre Modification on Dyeing. In: CEC Monograph Series, "Fibre-Grade Polymers, Chemical Fibres and Special Textiles", Vol. 1, Lódž, Poland 2001, 133-134
- [3]\* Hodul, P., Weberová, M., Marcinčin, A., Jedlovská, M.:  $\beta$ -cyklodextrine in textile finishing. In: CEC Monograph Series, "Fibre-Grade Polymers, Chemical Fibres and Special Textiles", Vol. 1, Lódž, Poland 2001, 79-85
- [4]\* Krištofič, M.: PA6/Copolyamides Fibre-Forming Blends. In: CEC Monograph Series, "Fibre-Grade Polymers, Chemical Fibres and Special Textiles", Vol. 1, Lódž, Poland 2001, 247-259
- [5]\* Marcinčin, A., Ujhelyiová, A., Hricová, M., Marcinčinová, T.: Modification of Polypropylene Fibres by Polymeric Additives. In: International Millenium Congress on Innovations in Fibre, Yarn Fabric Technology and Finishing, Terrassa, June 15-17, 2001, Spain
- [6]\* Borsig, E., Fiedlerová, A., Schulze, U., Pionteck, J.: Synthesis of IPN as a Method of Preparation of new Polymer Materials from Known Polymer Components. In: XV. Konferencja naukowa Modyfikacja polimerów Wroclaw 2001 87-90
- [7]\* Marcinčin, A., Ujhelyiová, A., Zemanová, E., Marcinčinová, T.: Mass pigmentation of polypropylene and polyethylene terephthalate fibres. In: Fibre Grade Polymers, Chemical Fibres and Special Textiles. Central European Conference Monograph Series Vol. 1, pp. 145-155, Lodz 2001, Poland
- [8]\* Marcinčin, A., Legéň, J., Hudecová, D., Marcinčinová, T., Šesták, J., Spevárová, E.: Antibacterial Chemical Fibres and Fibrous Materials, 1<sup>st</sup> Autex Conference "Technitex 2001" Technical Textile, Designing Textiles for Technical Application. Povoá de Varzim (Univerzity of Minho), June 26-29, 2001 Portugal
- [9]\* Marcinčin, A., Ujhelyiová, A.: Morphology and Properties of PP/LDPE and PP/PET Blend Fibres. In: CEC Monograph Series, "Fibre-Grade Polymers, Chemical Fibres and Special Textiles", Vol. 2, Bratislava 5. -7. 9. 2001, 244-251
- [10]\* Krištofič, M.: Copolyamides Based on  $\epsilon$ -caprolactam and Isophthalic Acid. In: CEC Monograph Series, "Fibre-Grade Polymers, Chemical Fibres and Special Textiles", Vol. 2, Bratislava 5. -7. 9. 2001, 252-255
- [11]\* Krištofič, M., Murárová, A.: Fibre- Forming Blends of Polar Polymers. In: CEC Monograph Series, "Fibre-Grade Polymers, Chemical Fibres and Special Textiles", Vol. 2, Bratislava 5. - 7. 9. 2001, 256-259
- [12]\* Murárová, A., Krištofič, M., Hodul, P., Jambrič, M.: The Influence of Cross-section of PET Fibres on Dyeing In: CEC Monograph Series, "Fibre-Grade Polymers, Chemical Fibres and Special Textiles", Vol. 2, Bratislava 5.-7. 9. 2001, 260-263
- [13]\* Pavlíková, S., Borsig, E., Marcinčin, A.: PP Nanocomposite Fibres. In: CEC Monograph Series, "Fibre-Grade Polymers, Chemical Fibres and Special Textiles", Vol. 2, Bratislava 5. - 7. 9. 2001, 275-279
- [14]\* Marcinčin, A., Zemanová, E., Marcinčinová, T., Brejka, O., Budzák, D.: Rheological Properties of Polyester Pigment Concentrates. In: CEC Monograph Series, "Fibre-Grade Polymers, Chemical Fibres and Special Textiles", Vol. 2, Bratislava 5. -7. 9. 2001, 290-294
- [15]\* Mlynarčíková, Z., Borsig, E.: Physical Properties of Polypropylene/Polyamide 6 Blend Fibres. In: CEC Monograph Series, "Fibre-Grade Polymers, Chemical Fibres and Special Textiles", Vol. 2, Bratislava 5. -7. 9. 2001, 295-298
- [16]\* Sroková, I., Ebringerová, A., Hodul, P.: Biopolymers from Polysaccharides. In: CEC Monograph Series, "Fibre-Grade Polymers, Chemical Fibres and Special Textiles", Vol. 2, Bratislava 5. -7. 9. 2001, 299-302
- [17]\* Legéň, J., Karabcová, N., Krištofič, M., Zemanová, E.: Blend Fibres Polypropylene/Polyethylene Terephthalate. In: CEC Monograph Series, "Fibre-Grade Polymers, Chemical Fibres and Special Textiles", Vol. 2, Bratislava 5. -7. 9. 2001, 346-348
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- [27]\* Murárová, A., Krištofič, M., Jambrich, M., Hodul, P.: Požiadavky na textilie pre odievanie. Requirements for textiles clothing In: Zborník príspevkov z 53. Zjazdu chemických spoločností, E-P14, Banská Bystrica, 3. - 6. 9. 2001, 73-74
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- [30]\* Fiedlerová, A., Borsig, E., Greco, R., Iavarone, M.: Optické vlastnosti PN systémov: PE/BMA-co-MMA. Optical properties of IPN-like networks PE/BMA-co- MMA. In: 53. zjazd chemických spoločností, Banská Bystrica, 3. - 6. 9. 2001, F-PO7, 80-81
- [31]\* Kósa, Cs., Danko, M., Fiedlerová, A., Hrdlovič, P., Borsig, E., Weiss, R. G.: Pyrenylová flouescencia ako značka pre štúdium štruktúry polyméru a difúzie v PE: poly(butylmetakrylát-co-polystyrén) obsahujúca vzájomne preniknutú sieť a príbuzné systémy. Pyrenyl fluorescence as a probe of polymer structure and diffusion in a polyethylene: poly(butylmethacrylate-co-polystyrene) interpenetrating network and related polymers. In: 53. zjazd chemických spoločností, Banská Bystica, 3. - 6. 9. 2001, F-PO13, 92
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- [33]\* Jambrich, M., Jambrich, P., Lučivjanský, J., Michlík, P., Murárová, A., Papajová, V., Revús, M.: The Development of Polypropylene Fibres in Slovakia. In: Proceedings I., 40<sup>th</sup> International Petroleum Conference, Bratislava, 17. - 19. 9. 2001, PE - 42
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### C. Books and Textbooks

### D. Patents

### E. Research Reports

## DEPARTMENT OF GRAPHIC ARTS TECHNOLOGY AND APPLIED PHOTOCHEMISTRY

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**Research Fellows:**  
Alžbeta Blažková, PhD, František Bednár, PhD (till 20.4.2001), Milena Reháková, PhD, Zuzana Jakubíková (from 1.10.2001), Jozef Fedák (civil service)

**PhD Students:**  
Ivana Lörinczová, Juraj Kindernay, František Belányi (from 1.10.2001)

**Technical Staff:**  
Mária Bardúnová, Alena Dušeková, Juraj Hamza (till 30.9.2001), Martin Kovalčík

### II. TEACHING AND RESEARCH LABORATORIES

#### A. Teaching Laboratories

Laboratory of Printing Technology  
Laboratory of Photochemistry and Photography  
Laboratory of Optical Spectroscopy and Photometry  
Laboratory of Thin Films and Plasma Technology  
Laboratory of Rheology

### III. TEACHING

#### A. Undergraduate Study

##### 6th Semester (spring)

|                               |         |  |
|-------------------------------|---------|--|
| Paper and Print, Graphic Arts | (2-2 h) | Krkoška (Dept. Wood, Paper, Pulp), Panák                             |
| Term Project                  | (0-4 h) | Blažková, Čeppan, Havlínová, Jančovičová,<br>Mikula, Panák, Reháková |

##### 7th Semester (autumn)

|                                   |         |   |
|-----------------------------------|---------|---|
| Colloids Systems and Interfaces   | (2-1 h) | Bakoš (Dept. Plastics and Rubber), Reháková |
| Polymer and Paper Physic          | (0-2 h) | Jančovičová                                 |
| Photochemistry and Photography I. | (2-1 h) | Čeppan, Reháková                            |
| Surface and Thin Film Technology  | (2-0 h) | Mikula                                      |
| Advanced Laboratory Course I.     | (0-9 h) | Havlínová, Jančovičová, Mikula, Reháková    |
| Typography and Text Processing    | (0-2 h) | Kindernay                                   |

##### 8th Semester (spring)

|                                    |         |  |
|------------------------------------|---------|--|
| Photochemistry and Photography II. | (2-0 h) | Čeppan                                     |
| Printing Technology I.             | (2-0 h) | Panák                                      |
| Advanced Laboratory Course II.     | (0-7 h) | Čeppan, Havlínová, Jančovičová, Lörinczová |
| Planning for Printing Production   | (0-2 h) | Panák                                      |

##### 9th Semester (autumn)

|                                 |          |  |
|---------------------------------|----------|--|
| Printing Technology II          | (2-0 h)  | Panák  |
| Repronc                         | (1-3 h)  | Mikula,  |
| Advanced Laboratory Course III. | (0-14 h) | Panák, Jakubíková, Blažková, Čeppan,<br>Havlínová, Jančovičová, Mikula, Reháková |



## IV CURRENT RESEARCH PROJECTS

### A. The study of relations between physical and chemical properties of the constituents and structures of printed images and image information quality in graphic arts technologies for planar polymer materials (Michal Čeppan)

1. Study of physical and chemical properties of macromolecular systems in constituents and structure of colour images on planar polymer materials. Characterization of optical properties of multiplayer structures of images by methods of objective microphotometry, spectrophotometry and colorimetry.
2. Study of influence of surface and rheological parameters of macromolecular systems of printing inks on the course of their transfer on planar polymer materials in the process of printed image formation.
3. Study of photochemical reactions of selected photopolymerization systems and their relation to the stability and quality of printed images.

### B. Coating thickness measurement of non-visible fluorescent UV colors (Contract with KASICO, a. s., printing house, Milan Mikula)

The effective layer thickness of a fluorescent UV sensitive color is not easy to control during a printing process. Classical densitometry cannot be applied because the fluorescent UV colors are non-visible. The problem was solved studying the fluorescent properties of the UV colors, their excitation and emission spectra. The prototype of a simple manual measuring system for technological application has been built up, based on appropriate excitation light source, detector, and applying the proper filtration of light. The prototype is now experimentally tested in the printing house.

### C. Thickness measurement of the fountain solution layer on lithographic plates (Contract with Ekotrading - Inkflow a.s., Bratislava, Milan Mikula, Michal Čeppan)

The measurement of a dampening level of wetted lithographic plates during offset printing process is important print quality factor that is not commonly under control. The known solution using IR absorption at 2.9 micrometers is demanding and expensive. The problem was solved by the measurement of the fountain solution film thickness of the non-image area on the real litho plate, online on form cylinder during the printing process in the printing machine. The principle used is based on the change of gloss with wetting, it means on the measurement of light specularly and diffusionaly reflected from the wetted plate. Experimental arrangement was created and tested in cooperation with Ekotrading - Inkflow a.s., Bratislava.

### D. Study of color shifts of prints on flexible packaging caused by adhesive laminating (Contract with Chemosvit, a.s., Michal Čeppan)

Adhesive laminating of flexible packaging materials changes gloss and overall appearance of the printed structures. Existence of thin metallic layer and primer interface cause significant and frequently unexpected and not easily predictable color shifts of prints. The goal of project was to map in the terms of color difference overall color changes of rotogravure prints on flexible packaging material caused by adhesive laminating by alumina foil.

## V. COOPERATION

### A. Cooperation in Slovakia

Chemosvit, Svit  
 Concordia Printing House, Bratislava  
 Inkflow-Ekotrading, Bratislava  
 Printing House BB, Banská Bystrica  
 Printing House Kasico, Bratislava

### B. International Cooperation

Technical University Brno, Faculty of Chemistry, Czech Republic  
 - Photochemical properties of light sensitive layers

### C. Membership in Domestic Organization and Societies

Slovak Union for Industrial Chemistry, Bratislava (M. Čeppan, B. Havlínová, M. Mikula, J. Panák, V. Dvonka, J. Fedák, V. Jančovičová, J. Kindernay, M. Reháková, I. Lörcinczová)

### D. Membership in International Organization and Societies

European Photochemistry Association (M. Čeppan)  
 International Society of Imaging Science and Technology, Springfield, USA (M. Čeppan)  
 Graphic Arts Technical Foundation, Sewickley, USA (M. Čeppan)

### G. Visitors from abroad

Dr. Michal Ďurovič State Central Archives in Prague, Czech Republic, June 2001 (2 days)  
 Dr. Ulrich Moosheimer Fraunhofer-Institut for Process Eng. And Packaging, Freising, Germany, November 2001 (1 day)  
 Dr. Wei Shen Australian Pulp and Paper Institute, Monash University, Australia (4 days)

### H. Visits of Staff Members and PhD Students to Foreign Institutions

M. Reháková State Central Archives in Prague, Czech Republic, January 2001 (2 days)

|  |   |
|--|---|
| A. Blažková, V. Bednár, M. Čeppan,<br>I. Panák, V. Jančovičová, M. Reháková,<br>J. Kindernay, I. Lörinczová, M. Kovalčík | Heidelberg Druck Maschinen, A.G., Heidelberg, Germany, March 2001<br>(5 days)   |
| B. Havlínová   | State Central Archives in Prague, Czech Republic, March 2001 (3<br>days)  |
| M. Čeppan  | Faculty of Chemistry, Technical University of Brno, Czech Republic,<br>May 2001 (2 days)                                |
| V. Jančovičová, B. Havlínová, A. Blažková,<br>M. Reháková, A. Dušeková, J. Kindernay,<br>I. Lörinczová, M. Kovalčík      | International Fair EMBAX 2001, Brno, Czech Republic, May 2001 (1<br>day)  |
| M. Čeppan, M. Mikula, J. Panák, M. Reháková  | 5 <sup>th</sup> Seminar on Graphic Arts Technology, University of Pardubice,<br>Czech Republic, September 2001 (3 days) |

## VI. THESES AND DISSERTATIONS

### A. Graduate Theses (MS Degree) for state examinations after five years of study (supervisors are written in brackets)

|                 |  |
|-----------------|--|
| Babiaková D.:   | The effect of accelerated aging on the stability of printing ink applied on a paper support. (B. Havlínová)      |
| Belányi F.:     | Study of changes of printed papers during accelerated aging. (B. Havlínová)                                      |
| Belešová Ľ.:    | Study of recording dyes properties and their affect on paper supports. (M. Ďurovič)                              |
| Burda V.:       | Study of photopolymeric reactions of monomer mixtures. (A. Blažková)   |
| Čellár D.:      | Automatized measurement of the wetting level of a printing plate. (M. Mikula)                                    |
| Čiernik R.:     | Preparation and properties of photochemically modified polymer layers. (V. Jančovičová)                          |
| Danko S.:       | Study of printability and adhesion properties of foils treated by surface discharge. (M. Mikula)                 |
| Halabicová M.:  | Study of photolysis of iodonium salt. (V. Jančovičová)   |
| Jakubíková Z.:  | Ink transfer and wetting in offset lithography. (J. Panák)   |
| Jurík M.:       | Study of the image structure resolution using imaging photometry. (M. Čeppan.)                                   |
| Kovalčíková M.: | Aging and aging evaluation of the salt graphic image. (M. Reháková)  |
| Malec B.:       | Study of accelerated light aging of graphical information. (M. Reháková)   |
| Plachý M.:      | Rheoviscosimetry of offset inks and their emulsions with fountain solutions. (J. Panák)                          |
| Studený P.:     | Study of colour changes during the treatment of printed packeging foils. (M. Čeppan)                             |
| Šuťáková S.:    | Preparation and properties of thin polymeric films using photopolymerization on different support. (A. Blažková) |

## VII. PUBLICATIONS

### A. Journals (\*registered in Current Contents)

- [1]\* Brunner R., Pinčík E., Mikula M., Záhora J.: Reflectance spectrometry of TiO<sub>2</sub> optical coatings on c-Si: The real data based simulation. *Acta Phys. Slov.* 51 (1) 17-26 (2001)
- [2]\* Kindernay J., Panák J., Mikula M.: Rheoviscometry of offset inks and their emulsions with water. *Chem. Pap.* 55 (1), 15-22 (2001)
- [3]\* Mikula M., Búc D., Pinčík E.: Electrical and Optical Properties of Copper Nitride Thin Films Prepared by Reactive DC Magnetron Sputtering. *Acta Phys. Slov.* 51, 35-43 (2001)
- [4] Panák J., Gonová O.: Reologia offsetowych farb arkuszowych. Część I. Rheology of sheet-fed offset inks (in Polish). Part I. *Poligrafika LIII* (2), 57–59, ISSN 0373-9864 (2001)
- [5] Panák J., Gonová O.: Reologia offsetowych farb arkuszowych. Część II. Rheology of sheet-fed offset inks (in Polish). Part II. *Poligrafika LIII* (3), 94–95; ISSN 0373-9864 (2001)
- [6] Panák J., Gonová O.: Reologia offsetowych farb arkuszowych. Część III. Rheology of sheet-fed offset inks (in Polish). Part III. *Poligrafika LIII* (4), 68–69, ISSN 0373-9864 (2001)

### B. Conferences (\*international conferences)

- [1] Čeppan M., Kosorín M., Mikula M., Pitoňák M.: Farebnosť potlače flexibilných obalov. Print Colourfulness of Flexible Packaging Materials (in Slovak). In: Proceedings of 4th Seminar on Graphic Arts Technology, Pardubice, Czech Republic, September 12.-13. 2001, p. 102-109, ISBN 80-7194-372-X
- [2] Havlínová B., Babiaková D., Mináriková J., Kindernay J.: Vplyv urýchleného starnutia na potlačenú podložku. The Effect of Accelerated Aging on Printed Support (in Slovak). In: Proceedings of Pulp and Paper – Technology, Properties and Enviroment, Bratislava, September 11.-12. 2001, p. 202-205, ISBN 80-227-1566-2

- [3] Havlínová B., Belányi F., Čeppan M., Reháková M.: Štúdium zmien potlačeného papiera počas urýchleného starnutia. Study of Printed Paper Changes During Accelerated Aging (in Slovak). In: Proceedings of 4th Seminar on Graphic Arts Technology, Pardubice, Czech Republic, 12.-13. 2001, p. 64-70, ISBN 80-7194-372-X
- [4] Jančovičová V., Karovičová I., Blažková A., Kindernay J.: Fotopolymerizácia vinyléterov iniciovaná organokovovou soľou. Photopolymerisation of Vinyl ethers Initiated by Organometallic Salt (in Slovak). In: Proceedings of 53th joint meeting of the Chemical Societies, Banská Bystrica, September 3.- 6. 9. 2001, ISBN 80-89029-24-8, p. 88-89
- [5] Karovičová I., Jančovičová V., Čiernik R., Čeppan M.: Fotochemicky modifikovateľné bariérové vrstvy na báze polyvinylalkoholu. Photochemically Modified Barrier Layer on the Polyvinyl Alcohol Base (in Slovak). In: Proceedings of 53th joint meeting of the Chemical Societies, Banská Bystrica, September 3.- 6. 9. 2001, ISBN 80-89029-24-8, p. 90-91
- [6] Kopáni M., Mikula M., Jergel M., Záhora J., Tucoulou R., Pinčík E.: About an Influence of Ar Ion Beam of Very Low Energy on a-Si:H Properties. In: Proceedings of 2th International Seminar on Semiconductor Surface Pasivation SSP 2001, Gliwice, Poland, 2001
- [7] Mikula M., Černák M.: Účinnejšia koróna pre predtlačovú úpravu polymérnych fólií. More Effective Corona for Prepress Treatment of Polymeric Foils (in Slovak). In: Proceedings of 4th Seminar on Graphic Arts Technology, Pardubice, Czech Republic, September 12.-13. 2001, p. 82-88, ISBN 80-7194-372-X
- [8] Mikula M., Reháková M., Kindernay J.: Urýchlené svetelné starnutie papiera a tlače pomocou nových svetelných zdrojov. Accelerated Aging of Papers and Prints Using New Light Sources (in Slovak). In: Proceedings of Pulp and Paper – Technology, Properties and Environment, Bratislava, September 11.-12. 2001, p. 198-201, ISBN 80-227-1566-2
- [9] Panák J., Plachý M.: Vplyv vlhčiaceho roztoku na viskozitné vlastnosti heatsetových farieb. The Effect of Fountain Solutions on Viscosity Properties of Heatset Inks (in Slovak). In: Proceedings of 4th Seminar on Graphic Arts Technology, Pardubice, Czech Republic, September 12.-13. 2001, p. 51-63, ISBN 80-7194-372-X
- [10] Reháková M., Malec B., Čeppan M., Mikula M.: Starnutie a hodnotenie starnutia grafických informácií. Aging and Aging Evaluation of Graphic Information (in Slovak). In: Proceedings of 4th Seminar on Graphic Arts Technology, Pardubice, Czech Republic, September 12.-13. 2001, p. 112-120, ISBN 80-7194-372-X
- [11] Szeiffová G., Havlínová B.: Porovnanie stálosti a trvanlivosti ofsetového, kancelárskeho, recyklovaného a ručného papiera. Comparison of Stability and Durability of Offset, Office, Recycled and Hand Made Papers (in Slovak). In: Proceedings of Pulp and Paper – Technology, Properties and Environment, Bratislava, September 11.-12. 2001, Bratislava, September 11.-12. 2001, p. 217-221, ISBN 80-227-1566-2

## DEPARTMENT OF INORGANIC CHEMISTRY

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**Associate Professors:**

Michal Dunaj-Jurčo, PhD; Mária Hvastijová, PhD, DSc; Marian Koman, PhD, DSc; Adela Kotočová, PhD; Anna Mašlejová, PhD; Ján Sýkora, PhD; Dušan Valigura, PhD;

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**Technical Staff:**

Viera Blažová; Andrea Bočová; Marta Danková; Valéria Habudová; Leonard Kováč; Silvia Markusová; Marta Polláková; Marta Sprušanská; Klára Valúchová;

### II. TEACHING AND RESEARCH LABORATORIES

**A. Teaching Laboratories:**

Laboratories of Practical Exercises

**B. Research Laboratories:**

Laboratory of Electrochemistry  
Laboratory of Photochemistry  
Laboratory of Magnetochemistry  
Laboratory of Thermal Processing  
Laboratory of Spectroscopy  
Laboratory of X-ray Analysis  
Laboratory of Powder Diffraction

### III. TEACHING

**A. Undergraduate Study**

**1st Semester (autumn)**

|                                    |         |   |
|------------------------------------|---------|---|
| Inorganic Chemistry I              | (3-2 h) | R. Boča, Kotočová, Melník, Šima, Valigura<br>Baloghová, M. Boča, Broškovičová, Dlháň,<br>Dunaj-Jurčo, Gembický, Hvastijová, Izakovič,<br>Jorík, Macášková, Makáňová, Mašlejová,<br>Mikloš, Moncol, Ondrejovičová, Palicová,<br>Papánková, Růžička, Segľa, Sirota, Sýkora,<br>Tatarko, Vančová, Vrbová |
| Inorganic Chemistry I (Laboratory) | (3 h)   |   |

**2nd Semester (spring)**

|                                     |         |   |
|-------------------------------------|---------|---|
| Inorganic Chemistry II              | (2-2 h) | Hvastijová, Koman, Melník, Ondrejovič, Sýkora<br>Baloghová, M. Boča, Broškovičová, Dlháň,<br>Gembický, Izakovič, Jorík, Macášková,<br>Makáňová, Mašlejová, Mikloš, Ondrejovičová,<br>Palicová, Papánková, Růžička, Segľa, Sirota,<br>Sýkora, Tatarko, Vančová, Vrbová |
| Inorganic Chemistry II (Laboratory) |         |   |

**7th Semester (autumn)**

|  |          |   |
|--|----------|---|
| Chemical Bond and Chemical Structure                   | (2-0 h)  | R. Boča                                       |
| Chemistry of Coordination and Organometallic Compounds | (2-0 h)  | Ondrejovič                                    |
| Inorganic Photochemistry                               | (2-0 h)  | Sýkora  |
| Inorganic Syntheses                                    | (2-0 h)  | Valigura                                      |
| Laboratory Practice in the Major I                     | (0-10 h) | R. Boča, Kotočová, Ondrejovičová, Ondrejovič, |

Růžička, Segľa, Sýkora, Valigura

**8th Semester (spring)**

|  |         |   |
|--|---------|---|
| Bioinorganic Chemistry   | (2-1 h) | Melník  |
| Crystallochemistry   | (2-0 h) | Dunaj-Jurčo   |
| Indirect Methods of Research Structural Studies of Inorganic Compounds | (2-2 h) | Mašlejová   |
| Inorganic Materials  | (2-0 h) | Koman   |
| Laboratory of Speciality   | (6 h)   |   |
| Laboratory Practice in the Major II                                    | (0-6 h) | Jorík, Mašlejová, Mikloš  |
| Reaction mechanisms of Inorganic Compounds                             | (2-0 h) | Šima  |
| Spectral Methods of Control Technological Processes                    | (2-2 h) | Segľa   |
| Technics of a Mixture Separation                                       | (2-2 h) | Valigura  |
| <b>9th Semester (autumn)</b>   |         |   |
| Bioinorganic Chemistry   | (2-1 h) | Melník  |
| Catalysis  | (2-0 h) | Ondrejovičová   |
| Chemistry of Coordination and Organometallic Compounds                 | (2 h)   | Ondrejovič  |
| Inorganic Materials  | (2-1 h) | Koman   |
| Laboratory of Speciality   | (10 h)  | Mikloš, Koman, Mašlejová, Ondrejovičová, Růžička, Šima, Valigura, Papánková |

**B. PhD Study****1st Semester**

|                                   |        |                     |
|-----------------------------------|--------|---------------------|
| Structure of Inorganic Substances | (30 h) | R. Boča, Ondrejovič |
| Recent Coordination Chemistry*    | (30 h) | supervisors         |

**2nd Semester**

|  |        |             |
|--|--------|-------------|
| Reaction Mechanisms of Inorganic Compounds | (30 h) | Šima        |
| Recent Coordination Chemistry*             | (30 h) | supervisors |

\* Studied and controlled individually in correspondence with the doctoral thesis.

**IV. CURRENT RESEARCH PROJECTS****A. New coordination compounds, their solid state structure, solution reactivity and applications (Milan Melník)**

Structural data of thousands coordination and organometallic compounds of copper, iron, tin and germanium were classified and analysed and significant structural correlations and generalisations were formulated. The results have been utilised for searching biologically active compounds and spectrally, electrically and magnetically attractive substances. The structure of a number of complexes was solved, the results were compared with their biological activity, which generally have higher activity than that of related uncomplexed compounds. Some of the results have been patented. Donor-acceptor properties of 24 ligands were quantified for proposing their behaviour in biocomplexes.

A specific theoretical and experimental procedure characterising the construction of coordination polymers was elaborated. Crystal structure determination of some copper and nickel complexes contributed to the optimisation of favourable conditions for reactions of ligands forming new compounds in the coordination sphere.

The basic factors influencing the relation between the wavelength of irradiation and the photoredox efficiency of iron complexes were formulated. It was found that by photolysis of copper complexes generated hydroxyl radical in solutions participates in photodegradation of some pollutants. The results can be applied to improve ecology.

**B. Induced transformations in coordination compounds (Roman Boča)**

New complexes of the transition metal central atoms with interesting magnetic properties have been synthesized: mono-, bi-, tri-, tetra- and pentanuclear complexes. In addition to their characterisation by a temperature dependence of the magnetic susceptibility, also the magnetisation measurement until fields of 5.5 T have been done.

For solid Fe(II) complexes the circumstances influencing the spin transition from the low-spin to the high-spin state (the spin crossover) have been investigated. Complexes of Fe(II) with the heterocyclic N-donor multidentate ligands have been synthesized; these exhibit the spin crossover above the room temperature. Namely, the system  $[\text{Fe}(\text{bzimpy})_2](\text{ClO}_4)_2$  shows  $T_c = 403 \text{ K}$  and it is perfectly reversible with the hysteresis width of 12 K. A new, combined model of the spin crossover has been outlined; it allows a description of the angled walls of the hysteresis loop.

The monograph "R. Boča: Theoretical Foundations of Molecular Magnetism (Elsevier, Amsterdam, 1999)." contributes to the theory of the molecular magnetism. Capabilities of the various experimental techniques were utilized: the single crystal and powder diffraction, VT-IR spectra, DSC susceptibility and magnetisation measurements, EXAFS, synchrotron powder diffraction, Moessbauer spectroscopy, etc.

**C. Development and applications of methods for picking out of talented students in small as well as in larger groups with respect to the needs of the Faculty of Chemical and Food Technology of the Slovak Technical University (Anton Sirota)**

A new version of a didactic creativity test in organic chemistry was tested in smaller groups of students. The test was proved to be sensitive and reliable enough for picking out talented students in higher courses of the Faculty of Chemical and Food Technology.

The research team elaborated a new statute of a special club named "SOCRATES" that gathers teachers and talented

students of the Faculty. When creating the club, the methods for picking out of talented students proposed by the research team, were applied and those experience and methods were used which have proved to be successful also at the secondary school level.

Some members of the research team prepared special examination and teaching texts and held lectures for students of the Summer School in Chemistry organized for talented secondary school students in July 2001. Moreover, several of them were involved into special training of the students who represented Slovakia at the 33rd International Chemistry Olympiad in July 2001 in Mumbai (India) and achieved the 15th place in the competition from among 55 countries of all over the world.

A new journal "Chemické rozhľady" for enhancement of chemistry teaching has been established and thanks to sponsors, it is distributed free of charge to all secondary schools in Slovakia. The editor-in-chief and his deputy are members of the research team.

Results of the research team were gathered in 23 reviewed papers (in Slovak) and published in journals. Besides that one plenary lecture was presented at the international conference on chemical education.

## V. COOPERATION

### A. Cooperation in Slovakia:

Department of Physical Chemistry, Slovak Technical University, Bratislava  
 Department of Organic Chemistry, Slovak Technical University, Bratislava  
 Department of Chemical Physics, Slovak Technical University, Bratislava  
 Department of Inorganic Technology, Slovak Technical University, Bratislava  
 Department of Microbiology, Biochemistry and Biology, Slovak Technical University, Bratislava  
 Department of Ceramics, Glass and Cement, Slovak Technical University, Bratislava  
 Institute of Medical Chemistry, Medical Faculty, Komensky University, Bratislava  
 Institute of Inorganic Chemistry, Slovak Academy of Science, Bratislava  
 Institute of Rheumatic Diseases, Piešťany  
 Department of Inorganic Chemistry, Faculty of Science UPJŠ, Košice

### B. International Cooperation:

Technical University, Vienna, Austria  
 - Magnetic properties in solids and solutions  
 York University, Toronto, Canada  
 - X-ray analysis of transitions and non-transitions metal atoms  
 University of Helsinki, Finland  
 - X-ray analysis of solid compounds  
 University of Joensuu, Finland  
 - X-ray analysis of copper(II) compounds  
 Martin-Luther University, Halle-Wittenberg, Germany  
 - Structure and physical properties of transition metal complexis with non-linear pseudohalides  
 Technical University, Darmstadt, Germany  
 - New magnetic materials  
 University of Wroclaw, Poland  
 - Magnetic and x-ray analysis

### C. Membership in Domestic Organizations and Societies:

Slovak Chemical Society  
 Czech and Slovak Society for Crystal Growth  
 Czech and Slovak Crystallographic Association  
 Regional Committee of Czech and Slovak Crystallographers  
 Crystallographic Society  
 EPA Slovakia National Group

### D. Membership in International Organizations and Societies:

Czech and Slovak Crystallographic Association,  
 Prague, Czech Republic (Dunaj-Jurčo, Jorík, Koman, Mikloš)  
 Member of International Union of Crystallography,  
 IUCr (M.Dunaj-Jurčo)  
 Member of European Crystallographic Committee,  
 EEC (M.Dunaj-Jurčo)  
 American Chemical Society, USA (M.Melník, J.Sýkora)  
 European Photochemistry Association, Switzerland (J.Sýkora, M. Izakovič, M. Tatarko)  
 Member of EPA Standing Committee, Switzerland (J.Sýkora)  
 EPA Local Treasurer, Switzerland (J.Sýkora)  
 Finland Chemical Society (M.Melník)  
 Member of MGMC Editorial Board, Brusel (M.Melník)  
 International Information Center of International  
 Chemistry Olympiads (A.Sirota)

### E. Tempus Programme:

### F. International Scientific Programmes:

Scientific & Technological Cooperation Between Germany (TU Darmstadt) and Slovakia (STU Bratislava): New magnetic materials

- R. Boča, H. Fuess

Scientific Cooperation Between Germany (MLU Halle) and Slovakia (STU Bratislava): Untersuchungen zur Struktur und Reaktivität von Übergangsmetallkomplexen nichtlinearer Pseudohalogenide - M. Hvastijová, L. Jäger

Scientific Cooperation Between Poland (Wrocław University) and Slovakia (STU Bratislava) ESF Project: Molecular Magnets.- R. Boča, M. Verdaguer, M. Melník, J. Mrozinski

### G. Visitors from Abroad:

|                    |   |
|--------------------|---|
| Prof. R. Grobelny  | University of Wrocław, Poland, June 2001 (3 days)     |
| Prof. J. Mrozinski | University of Wrocław, Poland, June 2001 (3 days)     |
| Dr. E. Náhalska    | University of Wrocław, Poland, June 2001 (3 days)     |
| Prof. H. Necefoglu | Kafkas University, Kars, Turkey, June 2001 (3 days)   |
| Prof. M. Sundberg  | University of Helsinki, Finland, June (2001) (5 days) |

### H. Visits of Staff Members and PhD Students to Foreign Institutions:

|               |  |
|---------------|--|
| V. Jorík      | University of Technology, Brno, Czech Republic, January 2001 (1 day)                         |
| M. Koman      | Crystallographical Society, Prague, Czech Republic, February 2001 (1 day)                    |
| M. Melník     | Masaryk University, Brno, Czech Republic, March 2001 (1 day)                                 |
| M. Ružička    | Physical Institute of Czech Academy of Sciences, Prague, Czech Republic, March 2001 (2 days) |
| R. Boča       | University of Bern, Bern, Switzerland, April 2001 (10 days)                                  |
| J. Šima       | Technical University, Vienna, Austria, April 2001 (1 day)                                    |
| P. Segľa      | Technical University, Vienna, Austria, May 2001 (1 day)                                      |
| D. Mikloš     | Technical University, Vienna, Austria, May 2001 (1 day)                                      |
| M. Melník     | Technical University, Vienna, Austria, June 2001 (1 day)                                     |
| R. Boča       | Technical University, Darmstadt, Germany, June 2001 (27 days)                                |
| J. Moncol'    | Crystallographical Society, Bedřichov, Czech Republic, June 2001 (5 days)                    |
| B. Papánková  | Technical University, Darmstadt, Germany, June 2001 (16 days)                                |
| L. Dlháň      | Technical University, Darmstadt, Germany, June 2001 (16 days)                                |
| M. Melník     | York University, Toronto, Canada, July 2001 (30 days)  |
| J. Šima       | University of Veszprém, Hungary, July 2001 (6 days)  |
| M. Gembický   | Martin-Luther University, Halle/Saale, Germany, July 2001 (62 days)                          |
| A. Sirota     | Homi Bhabha Center for Science Education, Mumbai, India, July 2001 (12 days)                 |
| R. Boča       | Technical University, Darmstadt, Germany, August 2001 (16 days)                              |
| M. Hvastijová | Martin-Luther University, Halle/Saale, Germany, September 2001 (7 days)                      |
| M. Melník     | University of Granada, Spain, November 2001 (5 days)   |
| R. Boča       | University of Mainz, Germany, December 2001 (3 days)   |
| A. Sirota     | University of Cambridge, England, December 2001 (4 days)                                     |

## VI. THESES AND DISSERTATIONS

### A. Graduate Theses (MS Degree) for state examinations after five years of study (supervisors are written in brackets):

#### B. Dissertations (PhD):

|              |  |
|--------------|--|
| M. Boča      | Variations of magnetic properties of complexes and coordination-conditioned structure modulation. (D. Valigura)              |
| M. Izakovič  | Photocatalytic properties of copper complexes and their applications. (J. Sýkora)  |
| M. Vrbová    | Coordination compounds of higher complexity on base of heterocyclic ligands. (R. Boča)                                       |
| M. Tatarko   | Photochemical aspects of Fenton reactions. (J. Sýkora)   |
| M. Gembický  | Polynuclear complexes of polydentate ligands. (R. Boča)  |
| D. Ondrušová | Study of metal dithiocarbamates and their influence on kinetics of vulcanisation of rubber mixtures. (E. Jóna)               |
| M. Pajtášová | Study of carboxylato copper(II) and carboxylato cobalt(II) complexes and their influence on rubber-metal adhesion. (E. Jóna) |
| M. Palicová  | Study of the structure, physical, chemical and biological properties of N-heterocyclic Cu(II)-carboxylates. (M. Melník)      |

#### D. Habilitation Theses:

|          |  |
|----------|--|
| P. Segľa | Reactions of nitriles in the coordination sphere of transition metal complexes |
|----------|--|

## VII. PUBLICATIONS

## A. Journals (\*registered in Current Contents)

- [1]\* Boča R., Boča M., Dlháň L., Falk K., Fuess H., Haase W., Jaroščík R., Papánková B., Renz F., Vrbová M., Werner R.: Strong Cooperativeness in the Mononuclear Iron(II) Derivative Exhibiting an Abrupt Spin Transition above 400 K. *Inorg. Chem.*, 40, 3025-3033 (2001).
- [2]\* Boča R., Dlháň L., Makáňová D., Mrozinski J., Ondrejovič G., Tatarko M.: Magnetic exchange coupling in tetranuclear copper clusters of the type  $[Cu_4(\mu_4O)Cl_{6-n}Br_nL_4]$ . *Chem. Phys. Lett.*, 344, 305-309 (2001).
- [3]\* Čík G., Šeršeň F., Dlháň L.: Electric conductivity of poly(3-dodecylthiophene) and its dependence on the conformational changes of polymer chains. *Czechosl. J. Phys.*, 51, 257-271 (2001).
- [4]\* Hvastijová M., Kohout J., Buchler J. W., Katzenmeier H. W., Kožíšek J., Didierjean C.: Crystallographic and spectroscopic evidence of O-bonding in 3d-metal dicyanomethanonitrite complexes. *Z. Naturforsch.*, 56b, 100-104 (2001).
- [5]\* Hvastijová M., Kohout J., Díaz J. G., Kožíšek J., Buchler J. W.: X-ray structural and spectroscopic investigation of cyanamidonitrate nickel(II) complexes with pyrazole type ligands. *Trans. Met. Chem.*, 26, 430-434 (2001).
- [6]\* Koman M., Babjak M., Gracza T., Glowiak T.: Absolute configuration of the newly formed asymmetric centre in (1R,5R,8S)-8-benzyloxy-2,6-dioxabicyclo[3.2.1]octan-3-one. *Acta Cryst., Sect E* o360-o361 (2001).
- [7]\* Koman M., Moncol J., Hudecová D., Dudová B., Melník M., Korabik M., Mrozinski J.: Study of copper(II) pyridine-2,6-dicarboxylates: Coordination and distortion isomers of  $[Cu(pydca)(H_2O)_2]$ . *Polish J. Chem.*, 75, 957-964 (2001).
- [8]\* Mašlejová A., Boča R., Dlháň L., Papánková B., Svoboda I., Fuess H.: Structure and zero-field splitting in bis(1,2-dimethylimidazole)bis(acetato) nickel(II) molecular complex. *Chem. Phys. Lett.*, 347, 397-402 (2001).
- [9]\* Melník M., Koman M., Moncol J., Glowiak T.: Crystal structure, spectral and magnetic behavior of copper(II)(5-chlorosalicylato)<sub>2</sub>(aqua)<sub>2</sub>. *J. Coord. Chem.*, 53, 173-179 (2001).
- [10]\* Mikloš D., Segľa P., Glowiak T.: Formation of N-2-hydroxyalkylpyridine-2-carboxamides in the coordination sphere of copper(II). The crystal and molecular structure of dibromo-bis-(N-2-hydroxypropylpyridine-2-carboxamidino-N,N')copper(II). *Inorg. Chem. Commun.*, 4, 66-71 (2001).
- [11]\* Mikloš D., Segľa P., Palicová M., Kopcová M., Melník M., Valko M., Glowiak T., Korabik M., Mrozinski J.: Synthesis spectral and magnetic properties, and crystal structures of copper(II)2-methylthionicotinate adducts with chelating ligands. *Polyhedron*, 20, 1867-1874 (2001).
- [12]\* Mojumdar S. C., Melník M., Jóna E., Enamullah M.: Preparation and properties of Mg(II) complexes with acetic acid and its derivatives. *Jornal Bangl. Sci.*, 14, 41-45 (2001) (1.0)
- [13]\* Moncol J., Koman M., Melník M., Glowiak T.: Copper(II) clofibrates, Part II. A two-dimensional coordination polymer of  $Cu(II)(clofibrate)_2(3\text{-pyridylmethanol})_2$ . *CrystEngComm*, 54, 1-3 (2001).
- [14]\* Ondrejovičová I., Vrábek V.: Synthesis, Spectra and Crystal Structure of Tetrakis (triphenylarsine oxide)iron(III)-μ-oxo-tribromoiron(III) tetrabromoferrate(III) – acetonitrile. *J. Coord. Chem.*, 56, 1-9 (2001).
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- [18]\* Ondrušová D., Koman M., Jóna E., Pajťášová M.: Cobalt(III) tris(N-ethyl-N-phenyldithio carbamate) *Acta Cryst.*, E57, m172-m173 (2001).
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- [20]\* Potočňák I., Dunaj-Jurčo M., Mikloš D., Jäger L.: Crystal structure of bis(2,2'-bipyridine-N,N')(dicyanamido-N)copper(II)tricyanomethanide electronic and structural parameters describing the shape of coordination polyhedra in five-coordinated copper (II) compounds. *Monat. Chem.*, 132, 315-327 (2001).
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- [22]\* Ružička M.: Metody rústu kryštáľů. *Československý časopis pro fyziku*, 51 107-115 (2001).
- [23]\* Šima J., Brezová V.: Mechanism of photoinduced processes in solutions of iodo iron(III) complexes containing Schiff Base ligands. *Monatshette für Chemie*, 132, 1493-1500 (2001).
- [24]\* Šima J., Lauková D., Brezová V.: Photoredox reactions of iodo ferric complexes containing tetradentate ligands, *Coll. Czech. Chem. Commun.*, 66, 109-118 (2001).
- [25]\* Šima J., Súkeník M.: Black holes – estimation of their lower and upper mass limits stemming from the model of expansive nondecelerative universe. *Spacetime and Substance*, 2, 79-81 (2001).
- [26] Šima J., Súkeník M.: Black holes – Estimation of their lower and upper mass limits stemming from the model of expansive nondecelerative universe. *Physic*, <http://xxx.lanl.gov/abs/physics/0109057> (2001).
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- [35] Sirota A.: Úlohy z anorganickej chémie (Tasks from inorganic chemistry). *Chemické rozhľady*, 3, 3–6 (2001).
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- [40] Súkeník M., Šima J.: Thermodynamics of expansive nondecelerative universe. *General Relativity and Quantum Cosmology*, <http://xxx.lanl.gov/abs/gr-qc/0106078> (2001).
- [41] Súkeník M., Šima J.: Wheeler-Feynman absorber theory viewed by model of expansive nondecelerative universe. *Physic*, <http://xxx.lanl.gov/abs/physics/0104066> (2001).
- [42] Valigura D.: Výpočty v systémoch rovnováh I. Rovnováha silných, málorozpustných elektrolytov, (Calculations in equilibrium systems I. Equilibrium in strong, slightly dissolving electrolytes). *Chemické rozhľady*, 1, 118-127 (2001).
- [43] Valigura D.: Výpočty v systémoch rovnováh II. Rovnováha v roztokoch silných málorozpustných elektrolytov v prítomnosti iného elektrolytu s rovnakým iónom (Calculations in equilibrium systems II. Equilibrium in solutions of strong and slightly dissolving electrolytes in the presence of another electrolyte with identical ion). *Chemické rozhľady*, 3, 27–36 (2001).

## B. Conferences (\*international conferences)

- [1] Balogová Z., Mazúr M., Valko M., Baran P., Dlháň L., Valigura D.: Structure and EPR spectra of 1:1 copper(II) complexes with 2,2-bipyridine-N,N-dioxide ligand. Proc. 18<sup>th</sup> International Conference on Coordination and Bioinorganic Chemistry, Smolenice, Slovakia (2001).
- [2] Boča R.: Novel aspects of spin crossover systems. Proc. 18<sup>th</sup> International Conference on Coordination and Bioinorganic Chemistry, Smolenice, Slovakia (2001).
- [3] Diáz J. G., Hvastijova M., Kožíšek J.: Cyanamidonitrate-copper(II), nickel(II) and cobalt(II) complexes of imidazole and pyrazole ligands. 20<sup>th</sup> ECM, Krakow, Poland (2001).
- [4] Dlháň L., Gembický M., Boča R., Renz F.: A heptanuclear iron(II)-iron(III) system with twelve unpaired electrons. Development of Materials Science in Research and Education, Kežmarské Žľaby, Slovakia (2001).
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- [10]\* Hudecová D., Uher M., Koreňová A., Melník M., Brtko J.: Deriváty kyseliny kojovej – perspektívny zdroj bioaktívnych zlúčenín využiteľných v ochrane rastlín. 53. Zjazd chemických spoločností, Banská Bystrica, Slovakia (2001).
- [11] Hvastijová M., Kohout J., Kožíšek J., Jäger L.: Cyanamidonitrate complexes of Ni(II), Co(II) and Cu(II) with pyrazole ligands; nucleophilic addition in the Cu(II) coordination sphere. Proc. 18<sup>th</sup> International Conference on Coordination and Bioinorganic Chemistry, Smolenice, Slovakia (2001).
- [12] Jorík V.: Spresnenie štruktúry hydratovaného zeolitu NaY – TOF neutrónové dáta. Regionálna prášková difrakčná konferencia RPDK (2001), Liptovský Mikuláš, Slovakia (2001).
- [13] Koman M., Melník M., Hudecová D., Moncof J., Dudová B., Glowiak T.: Crystal structure of copper(II) clofibrates with some derivatives of pyridine and their biological activity. Challenges for Coordination Chemistry in the New Century, Slovak Technical University Press, Bratislava, Slovakia (2001).
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- copper(II) complexes. Challenges for Coordination Chemistry in the New Century, Slovak Technical University Press, Bratislava, Slovakia (2001).
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### C. Books and Textbooks

- Holloway C. E., Melník M.: Heterometallic tin compounds: classification and analysis of crystallographic and structural data. Part I. Dimeric derivatives. *M.G.M.C.*, 24, 133-194 (2001).
- Holloway C. E., Melník M.: Heterometallic tin compounds: classification and analysis of crystallographic and structural data: Part II. Trimeric to polymeric derivatives. *M.G.M.C.*, 24, 467-581, (2001).
- Holloway C. E., Melník M.: Germanium coordination compounds: classification and analysis of crystallographic and structural data. *M.G.M.C.*, 24, 681-726 (2001).

#### D. Patents

- [1] Brtko J., Hudecová D., Ficková M., Melník M., Uher M.: Komplexy 5-hydroxymetyl a 5-hydroxy-2-chlórmetyl-4H-pyrán-4-ónu a spôsob ich prípravy. PV 1726 (2001).

## DEPARTMENT OF INORGANIC TECHNOLOGY

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### I. STAFF

**Full Professors:**

Pavel Fellner, PhD, DSc;

**Associate Professors:**

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**Assistant Professors:**

Ján Híveš, PhD; Anna Žúžiová, PhD;

**Research Fellows:**

Peter Adamčík; Vladimír Danielik, PhD; Vladimír Khandl; Matilda Zemanová, PhD;

**PhD Student:**

Michal Korenko; Marta Baníková;

**Technical Staff :**

Viliam Cauner; Eva Dekanová; František Kollár;

### II. TEACHING AND RESEARCH LABORATORIES

**A. Teaching Laboratories:**

Molten Salt Chemistry Laboratories  
Laboratories of Chemical Inorganic Syntheses and Industrial Inorganic Chemistry

**B. Research Laboratories:**

Molten Salt Chemistry and Electrochemistry Laboratories  
Technical Electrochemistry Laboratories  
Electroplating, Special Coatings and Corrosion Laboratories

### III. TEACHING

**A. Undergraduate Study**

1. Introductory courses

**3rd semester (autumn)**

|  |         |   |
|--|---------|---|
| Fundamental Principles of Inorganic Technology | (2-2 h) | Fellner, Adamčík, Danielik, Gabčová,<br>Chovancová, Korenko, Valtýni, Žúžiová |
|--|---------|---|

**5th semester (autumn)**

|  |         |                               |
|--|---------|-------------------------------|
| Corrosion and Material Surface Treatment | (2-0 h) | Chovancová                    |
| Laboratories of Corrosion                | (0-2 h) | Chovancová, Adamčík, Zemanová |

2. Advanced courses

**7th semester (autumn)**

|                                   |         |   |
|-----------------------------------|---------|---|
| Phase Equilibria                  | (2-1 h) | Gabčová, Fellner                                |
| Applied Thermodynamics            | (2-2 h) | Fellner, Danielik                               |
| Corrosion and Material Protection | (2-2 h) | Chovancová, Zemanová                            |
| Laboratories I.                   | (0-4 h) | Adamčík, Gabčová, Híveš, Chovancová,<br>Žúžiová |

**8th semester (spring)**

|                               |         |   |
|-------------------------------|---------|---|
| Chemical Reaction Engineering | (2-2 h) | Valtýni, Híveš                                |
| Applied Electrochemistry      | (2-1 h) | Híveš, Fellner                                |
| Laboratories II.              | (0-8 h) | Danielik, Gabčová, Híveš, Chovancová, Žúžiová |

**9th semester (autumn)**

|                                |          |  |
|--------------------------------|----------|--|
| Fertilizers                    | (2-0 h)  | Žúžiová, Gabčová   |
| Electrochemical Engineering    | (2-0 h)  | Híveš, Fellner   |
| Elements of System Engineering | (1-1 h)  | Valtýni, Danielik  |
| Laboratories III.              | (0-10 h) | Danielik, Fellner, Gabčová, Híveš, Chovancová,<br>Valtýni, Zemanová, Žúžiová |

**B. PhD Study**

|   |      |         |
|---|------|---------|
| Inorganic Technology and Materials Subjects | (4h) | Fellner |
|---|------|---------|

## IV. CURRENT RESEARCH PROJECTS

### A. Thermodynamics and Kinetics of the Processes on the Phase Boundary Aluminium – Melt (Pavel Fellner)

Equilibrium contents of sodium, lithium and calcium in aluminium in contact with the melts of the system  $\text{Na}_3\text{AlF}_6 - \text{AlF}_3 - \text{Al}_2\text{O}_3 - \text{LiF} - \text{CaF}_2$  were obtained in the temperature range 950°C – 1030 °C. A thermodynamic model describing the experimental data on the contents of alkali and earth alkaline metals in the aluminium cathode in aluminium electrolysis was developed.

The cathodic concentration overvoltage in  $\text{Na}_3\text{AlF}_6 - \text{AlF}_3 - \text{Al}_2\text{O}_3$  melts was investigated. The melts contained 10 and 20 mass % of  $\text{AlF}_3$ . Experimental data on the cathodic overvoltage agreed well with the values calculated from the content of sodium in aluminium. It was found that the addition of 5 mass %  $\text{CaF}_2$  or 5 mass %  $\text{MgF}_2$  does not influence the overvoltage significantly, while the addition of 2 mass %  $\text{LiF}$  decreases the overvoltage by 20 mV at a cathodic current density of 0.25 A.cm<sup>-2</sup> and by 50 mV at 0.75 A.cm<sup>-2</sup>.

### B. Preparation and Properties of Oxide Layers on Aluminium (Marta Chovancoová)

Composite material on the aluminium formed by the anodic oxidation of the aluminium in the acid electrolyte and alumina layer prepared by the usage of sol-gel method increased the application ability of the aluminium (corrosion resistance, decorative properties).

The ways of the anodic aluminium sealing were compared (hydrothermal sealing, cold impregnation, method sol-gel and sealing by the PTFE dipping) by the corrosion tests and EIS measurements in the wide frequency range.

The growth of the oxide layer at the defined conditions have been studied in the galvanostatic regime in the four mixed electrolytes on the basis of the sulfuric acid solution in the dependence on time, current density, temperature and electrolyte composition.

The hard composite coatings were reached by the electrochemical way on the basis of the iron matrix and dispersed silicium particles as well the ultrahard ceramics on the basis of the polysilazanes.

## V. COOPERATION

### A. Cooperation in Slovakia

Institute of Inorganic Chemistry Slovak Academy of Science, Bratislava

Department of Electrotechnology, Faculty of Electrical Engineering and Information, Slovak University of Technology in Bratislava, Bratislava

Department of Chemical Machines and Equipment, Faculty of Mechanical Engineering, Slovak University of Technology in Bratislava, Bratislava

### B. International Cooperation

Department of Applied Electrochemistry, Norwegian University of Science and Technology, Trondheim, Norway

- formation of carbides in aluminium electrolysis
- mechanism of anodic reaction in aluminium electrolysis
- inert anodes and anode effect in aluminium electrolysis
- behavior of sulfur and sulfur compounds in aluminium electrolysis
- contents of impurities in polarized aluminium in contact with cryolite-based melts

Technische Hochschule Darmstadt, Darmstadt, Germany

- infiltration of alumina by polysilazane Ceraset

Fachhochschule Münster, Germany

- ceramic superconductors

### C. Membership in Domestic Organizations and Societies

Union of Slovak Scientific and Technological Societies

Slovak Chemical Society

Fellner, Híveš, Gabčová, Chovancoová, Valtýni, Žúžiová

Fellner, Híveš, Gabčová, Chovancoová, Valtýni, Žúžiová, Danielik, Zemanová

Slovak Society for Surface Treatment and Technology

Fellner, Chovancoová

Slovak Cleaner Production Center

Chovancoová

### Membership in International Organizations and Societies

International Society of Electrochemistry

Híveš

EFCE Electrochemical Engineering

Fellner

### E. Tempus Programs

SOCRATES Programme: Higher Education (ERASMUS)

Student mobility, cooperation with Fachhochschule Münster, Germany.

Four Students worked in the laboratories of Material Science for three months.

### F. International Scientific Programs

### G. Visitors from Abroad

Prof. J. Thonstad

NTNU, Trondheim, Norway, May 2001 (1 week)

### H. Visits of Staff Members and Postgraduate Students in Foreign Institutions

P. Fellner

NTNU Trondheim, Norway, September 2001 (2 weeks)

|               |  |
|---------------|--|
| J. Híveš      | NTNU Trondheim, Norway, January 2001 (1 month), August 2001 (2 months)       |
| M. Korenko    | NTNU Trondheim, Norway, September 2001 (2 months)                            |
| M. Zemanová   | Technische Hochschule Darmstadt, Darmstadt, Germany, February 2001 (1 month) |
| M. Chovancová | ČVUT Prague, Czech Republic, February 2001 (1 day)                           |

## VI. THESES AND DISSERTATIONS

### A. Graduate Theses (MS Degree) for state examinations after five years of study (Supervisors are written in brackets):

|                      |   |
|----------------------|---|
| Marta Baníková:      | Investigation of content of iron and sulphur in cryolite-based melt. (Jana Gabčová)                             |
| Agáta Dráčová:       | Correlation between conditions of preparation and properties of oxide layers. (Matilda Zemanová)                |
| Henrieta Hanáková:   | Investigation of phase diagram of the system NaCl - KCl - KF. (Vladimír Danielik)                               |
| Blažej Horváth:      | Study of hydroxyapatites as selective catalysator for oxidation. (Milan Hronec)                                 |
| Martina Charišová:   | Preparation and study of physico-chemical properties of complex compounds on the basis of copper. (Peter Segľa) |
| Blanka Kubíková:     | Ceramics based on Al <sub>2</sub> O <sub>3</sub> for cutting tools. (Zdeněk Pánek)                              |
| Marián Kucharík:     | Study of solidus-liquidus equilibria of the system NaCl - NaF - KF. (Jana Gabčová)                              |
| Miroslav Moric:      | Preparation of composite coatings. (Ján Híveš)  |
| Daniela Repáňová:    | NPS liquid fertilizer of 9 : 11 : 6S type. (Jozef Papp)   |
| Zuzana Spišiaková:   | Study of vanadium impurities circulation in aluminium electrolytic cell. (Marta Chrenková)                      |
| Blanka Tkacziková:   | Time dependence of anodic coatings sealed by the combined method. (Marta Chovancová)                            |
| Tomáš Trcka:         | Carbothermic preparation of sialons. (Zoltán Lenčes)  |
| Jozef Vincenc Oboňa: | Phase equilibria in the system NaCl - KCl - BaCl <sub>2</sub> . (Vladimír Danielik)                             |
| Adriana Vyjidáková:  | Study of Cu(II) complexes. (Marián Koman)   |
| Jarmila Cibulková:   | Treatment of alkaline waste water. (Pavel Fellner)  |

### B. Dissertations (PhD):

### C. Dissertations (DSc):

### D. Habilitation Theses:

|                 |  |
|-----------------|--|
| Ján Híveš, PhD: | Electrochemical Processes in Aluminium Electrolysis. |
|-----------------|--|

## VII. PUBLICATIONS

### A. Journals (\*registered in Current Contents)

- [1]\* Danielik V., Gabčová J.: Phase diagram of the Na<sub>3</sub>AlF<sub>6</sub> - NaF - Na<sub>2</sub>SO<sub>4</sub>. *Thermochimica Acta* 366, 79 - 87 (2001)
- [2]\* Fellner P., Híveš J., Korenko M., Thonstad J.: Cathodic overvoltage and the contents of sodium and lithium in molten aluminium during electrolysis of cryolite-based melts. *Electrochimica Acta* 46, 2379-2384 (2001)
- [3]\* Thonstad J., Rolseth S., Rodseth J., Tonheim J., Danielik D., Fellner P., Híveš J.: The Content of Sodium in Aluminium in Laboratory and in Industrial Cells. *Light Metals* 2001, 441 - 447 (2001)
- [4]\* Híveš J., Korenko M., Fellner P.: Fe - Si Composite Coatings. *Chem. Papers* 55 (2), 81 - 85 (2001)
- [5]\* Chrenková M., Danielik V., Silný A., Daněk V.: Phase Diagram of the System KF - KCl - KBF<sub>4</sub> - K<sub>2</sub>TiF<sub>6</sub>. *Chem. Papers* 55 (2), 75 - 80 (2001)

### B. Conferences (\*international conferences)

- [1]\* Fellner P., Danielik V., Híveš J., Thonstad J.: The Relationship between the Cathodic Overvoltage and the Contents of Alkali and Earth Alkaline Metals in Aluminium During Electrolysis. In: *Proceedings of Eleventh International Aluminium Symposium, Trondheim September 19 - 22, 2001*, pp. 89 - 96
- [2]\* Híveš J., Lorentsen O. A., Thonstad J.: Inert Anode under Electrochemical Impedance Spectroscopy Study. In: *Proceedings of Eleventh International Aluminium Symposium, Trondheim September 19 - 22, 2001*, pp.137 - 143
- [3]\* Fellner P., Danielik V., Híveš J., Thonstad J.: The Contents of Alkali and Earth Alkaline Metals in the Aluminium Cathode in Aluminium Electrolysis. In: *Proceedings of 6th International Symposium on Molten Salt Chemistry and Technology, Shanghai, China, October 8 - 13, 2001*, pp. 114 - 117, ISBN 7-81058-391-3
- [4]\* Chrenková M., Danielik V., Van V., Fellner P., Daněk V.: Structure and Properties of the LiF-NaF-K<sub>2</sub>NbF<sub>7</sub> Melts. In: *Proceedings of 6th International Symposium on Molten Salt Chemistry and Technology, Shanghai, China, October 8 - 13, 2001*, pp. 86 - 93, ISBN 7-81058-391-3
- [5] Chovancová M., Zemanová M., Híveš J., Fellner P., Grmanová I.: Corrosion of the Steel Materials in the Model Soil Electrolytes. In: *Proceedings of 12th International Conference Korózia úložných zariadení, Košice, 29. - 30. May 2001*, pp. 11 - 15, ISBN 80-7099-582-3
- [6] Danielik V., Híveš J., Gabčová J.: Katódové napätie pri elektrolýze kryolitových tavenín. Cathodic overvoltage in aluminium

- electrolysis. (in Slovak) In: Proceedings of 53. zjazdu chemických spoločností, Banská Bystrica, 3. - 6. September 2001, pp. 193-194, ISBN 80-89029-23-X
- [7] Híveš J., Korenko M., Fellner P.: Elektrochemické kompozitné povlaky typu Fe – Si. Electrochemical composite coatings based on Fe – Si. (in Slovak) In: Proceedings of 43. medzinárodnej galvanickej konferencie, Bratislava 26. - 27. June 2001, pp.59 – 64
- [8] Chrenková M., Daněk V., Fellner P.: Elektrolytické pokovovanie v taveninách. Electrodeposition of metals in melts. (in Slovak) In: Proceedings of 43. medzinárodnej galvanickej konferencie, Bratislava 26. - 27. June 2001, pp. 70 – 74
- [9] Zemanová M., Chovancová M.: Chromátovanie zinkových povlakov. Chromating of zinc coatings. (in Slovak) In: Proceedings of 43. medzinárodnej galvanickej konferencie, Bratislava 26. - 27. June 2001, pp. 54 – 58
- [10]\* Korenko M., Baníková M., Fellner P., Gabčová J., Thonstad J.: A Preliminary Study of the Dissolution of FeS in Cryolite Melts. In: Proceedings of Eleventh International Aluminium Symposium, Trondheim September 19 - 22, 2001, pp. 281
- [11]\* Danielik V., Híveš J.: Cathodic Overvoltage and the Content of Sodium in Molten Aluminium During Electrolysis of Cryolite Based Melts. In: Proceedings of Molten Salts : From Fundamental to Applications, Kas, Turkey 4-14 May 2001, pp. P14
- [12]\* Zemanová M., Nemčeková K., Chovancová M.: Corrosion Properties of Teflon Sealed Anodized Aluminium. In: Proceedings of 6th International Conference Theoretical and Experimental Problems of Materials Engineering, Púchov September 5 - 7, 2001, pp. 31

### C. Books and Textbooks

- [1] Thonstad J., Fellner P., Haarberg G., M., Híveš J., Kvande H., Sterten A.: Aluminium Electrolysis. Fundamentals of the Hall - Héroult Process. Aluminium-Verlag, Marketing & Kommunikation GmbH, Düsseldorf, Germany, pages 359 (2001), ISBN 3-87017-270-3

### D. Patents

- [1] Zemanová M., Fellner P., Chovancová M., Koštenská I.: Spôsob prípravy tenkých vrstiev oxidov na hliníku a hliníkových zliatinách. The method of preparation of thin oxide layers on aluminium and aluminium alloys. (in Slovak) SK 281503 (9. 4. 2001)

## DEPARTMENT OF LANGUAGES

**Head of the Department:**  
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### I. STAFF

**Assistant Professors:**

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**Technical Staff:**

Katarína Vépyová;

### II. TEACHING AND RESEARCH LABORATORIES

English language classroom  
German language classroom  
Computer-operated Data Video Projector Room

### III. TEACHING

#### A. Undergraduate Study

The English language represents a compulsory subject for each student of this faculty. In special cases, if a student has a better knowledge of a different world language, he may ask the dean to be given permission to take up one of the following languages: German, French, Spanish, Russian or Italian. A prerequisite of the latter case is the intermediate level in the chosen language. The programme is taught in two semesters in the first year of the study and ended with a 4-credit exam. The objective of the language study is not to teach the general language, but the language for specific – prospective professional purposes. It means the participants will be able to use the language in the study of their specialist area literature, to further develop all the language skills actively with the aim of mastering extensive reading and listening to texts, academic writing, poster and conference skills, etc. In the final exam students are expected to prepare a poster, present and support it with arguments in a discussion. The long-term aim is to finally enable all faculty graduates to present - at least - the essential part of their thesis in the state exams also in a foreign language.

In case of a student who does not speak any of the above languages, he may take up an elementary course in English first and then study the compulsory technical language in the second, or possibly the third year of the study.

The students who have chosen a different language than English in the first year, will have to pursue English in three more terms after passing the exam in their first foreign language.

Foreign students have a 2-term course of the Slovak language.

Besides the above - mentioned compulsory courses there is a wide range of recommended subjects offered, such as English conversation, preparatory courses for beginners, remedial courses of various levels, German, Russian and so on, according to the interest of students in the current year; these are also available to SUT employees.

#### B. PhD Study

Postgraduate students are offered optional seminars for technical English (2-4 hours per week) in which they are taught academic skills, such as presentation techniques, writing reports, abstracts, summaries, solving case studies, etc. Postgraduates are obliged to pass an examination in which they defend their scientific work results, prove their communication, discussion and other academic skills in English. The subject is taught by Alžbeta Oreská, Veronika Polóniová, Zuzana Štefanovičová and Magdaléna Horáková.

### IV. CURRENT RESEARCH PROJECTS

#### A. Aspects of Teaching a Foreign Language for Specific Purposes at the University of Technology (Milan Kozlík)

The objective is to develop high quality course programmes tailored to the needs of our students.

Current results are:

- collection of new or adapted texts
- exploitation of our own reading materials from the department's material bank
- devising new, more challenging tasks for the newly acquired materials
- unit design
- discussion and evaluation of the newly adopted units
- implementing new forms of active and independent learning (e.g. Critical thinking in reading and writing in ESP)
- introduction of "Effective Presentation" and "Socializing" video programmes into teaching successful poster presentations for undergraduate and postgraduate students
- presenting more challenging topics from science and technology in the annual faculty competition "Student Research Activities"
- further continual teaching staff development in methodology and informatics.



## V. COOPERATION

### A. Cooperation in Slovakia:

- (1) Language departments within the Slovak University of Technology, Bratislava, and those of the Technical University, Košice: - joint project of preparing syllabuses for language state exam courses administered by SUT language departments which will - besides the general language- introduce also the area of scientific English;
- (2) Cooperation with IASTE: oral interviews with applicants for mobility abroad (A. Oreská, V. Polóniová)
- (3) Language section of the annual "ŠVOČ" (Students' Scientific and Research Activity) competition (16 May 2000)
- (4) Slovak Association of Translators and Interpreters (Polóniová)
- (5) Language Department of the Civil Engineering Faculty: a joint workshop on "Critical Thinking in Teaching Languages " (6 December 2001)

### B. International Cooperation:

CASAJC – Slovak and Czech Association of Language Centres in Higher Education (Polóniová – committee member)

### C. Membership in Domestic Organizations and Societies:

Slovak Association of Translators and Interpreters, Bratislava

Polóniová

### D. Membership in International Organizations and Societies:

British Council - Resource Centre, Bratislava

Oreská, Horáková

CERCLES – European Confederation of Language Centres in Higher Education

Polóniová

### International Scientific Programmes:

European Portfolio: A Language Passport to Unify Language Testing in Higher Education

Project promoter: Cercles/ CASAJC (Polóniová – team member)

## VII. PUBLICATIONS

- (1) Štefanovičová Z: Humour – the Spice of ELT. English Teaching Forum , Volume 39, July 2001, Washington D. C. 20520

### B. Conferences

- (1) Oxford University Press : On Teaching English in Slovakia (Oreská, Štefanovičová, 6 October 2001, Bratislava)

### C. Books and Textbooks

- (1) Oreská A., Harmanová M., Horáková M., Karvašová K., Kozlík M., Polóniová V., Štefanovičová Z.: English for Chemists. STU Publishing House, Bratislava 2001, ISBN 80-227-1543-3

## DEPARTMENT OF MANAGEMENT

### Head of the Department:

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### I. STAFF

#### Associate Professors:

Agáta Ďurkovičová, PhD, Marta Šostroneková, PhD

#### Assistant Professors:

Dušan Baran, PhD; Štefan György, PhD; Pavel Herzka, PhD; Dušan Hesek, PhD; Dušan Špirko, PhD; Peter Velický, PhD

#### Assistant Lecturers:

Martin Jozefček, Jana Kajanová, Monika Zatrochová

#### Technical Staff:

Martin Mikloš, Lýdia Hadrbulcová, Katarína Macušková

### II. TEACHING AND RESEARCH LABORATORIES

#### A. TEACHING LABORATORIES:

Laboratory of Computerized Technique

### III. TEACHING

#### A. Undergraduate Study

##### 1st semester

|           |         |         |
|-----------|---------|---------|
| Economics | (2-0 h) | Velický |
|-----------|---------|---------|

##### 2nd semester

|  |         |        |
|--|---------|--------|
| Fundamentals of Environmental Philosophy | (2-0 h) | Špirko |
|--|---------|--------|

##### 5th semester

|  |         |              |
|--|---------|--------------|
| Fundamentals of Management of Chemical and Food-Processing Enterprises | (2-2 h) | Šostroneková |
|--|---------|--------------|

|           |         |                       |
|-----------|---------|-----------------------|
| Marketing | (2-2 h) | Ďurkovičová, Garajová |
|-----------|---------|-----------------------|

##### 6th semester

|                     |         |                           |
|---------------------|---------|---------------------------|
| Introduction to Law | (2-0 h) | György                    |
| Semestral Project   | (0-4 h) | Ďurkovičová, Šostroneková |
| Accounting          | (2-2 h) | Šostroneková, Kajanová    |

##### 7th semester

|                         |         |          |
|-------------------------|---------|----------|
| Theory of a Firm        | (2-2 h) | Herzka   |
| Operations Research     | (3-2 h) | Hesek    |
| Strategic Management    | (3-2 h) | Jozefček |
| Calculations and Prices | (2-2 h) | Kajanová |

##### 8th semester

|  |         |             |
|--|---------|-------------|
| Capital Market and Enterprise Finances | (2-0 h) | Baran       |
| Marketing                              | (2-0 h) | Ďurkovičová |
| Decision-Making in Business            | (2-3 h) | Hesek       |
| Human Resource Management              | (2-2 h) | Herzka      |
| Production Management                  | (2-3 h) | Zatrochová  |

##### 9th semester

|  |         |                           |
|--|---------|---------------------------|
| Financial Management                         | (3-2 h) | Šostroneková              |
| Analysis of Enterprise Economy               | (3-2 h) | Baran                     |
| Logistics                                    | (2-2 h) | Jozefček                  |
| Fundamentals of Mercantile and Financial Law | (2-0 h) | György                    |
| International Marketing                      | (2-2 h) | Ďurkovičová               |
| Year's Project                               | (0-4 h) | Ďurkovičová, Šostroneková |

### IV. CURRENT RESEARCH PROJECTS

#### A. Modern conceptions of the basic orientation of the firm's strategic management (Agáta Ďurkovičová)

Part B: Strategic marketing and the organization of marketing.

At the present time characterized by permanent changes in the business activity marketing as an instrument of management is an inevitable prerequisite for the successful business. The knowledge and ability to employ the marketing appropriately permits enterprises to recognize in advance the market environment in which they operate. On the basis of the knowledge of this environment an enterprise is able to make correct decisions about its future position in the market. The marketing analysis belongs to basic marketing activities in conjunction with the management and provides information for other marketing-management activities.

An objective of this research stage is to perform the marketing analysis of the specific market segment, i.e. polymer-bonded rubber chemicals directed at finding the product's perspective in terms of the present as well as future market requirements. The results of this research should serve as a basis for the formation of the enterprise marketing strategy.

The research work consists of 5 chapters which are divided into several sections. In the first part, attention is paid to the definition of the marketing presented as an instrument of management and to the position of the marketing analysis in the marketing management. The second part is aimed at the market and its segmentation. Here the specific market segment of the polymer-bonded rubber chemicals, the choice of target groups, and the market position are characterized. The third part provides an external analysis comprising the analysis of the microenvironment and that of the industrial environment. The fourth part is focused on the internal analysis of the enterprise where the financial and technological factors, enterprise organizational structure, and enterprise competitive position are elaborated. In the last part of the work, the results of the marketing analysis incorporating the SWOT analysis as a synthesizing instrument of the results obtained from the internal and external analysis of the enterprise are evaluated.

## **B. Philosophical-social aspects of macroeconomic theories, the environmental, ethical and legal dimensions of engineering-technological and economic activities with regard to their specificities in the chemical and food-processing industry (Dušan Špirko)**

Part B: Genesis and development of views on the culture-nature relationship. Humanization strategies and environment. An engineer's environmental and social responsibility. Legal aspects of the business risk. Philosophical fundamentals of management.

Scientific objectives of the 2-nd stage of works in 2001 are following:

Completion of the analysis of genesis and the development of views on the relations of nature in the European cultural tradition.

Analysis of the principles of current humanization strategies in relation to the environment.

Study of principles of the engineer's social and environmental responsibility.

Social-psychological, political and environmental consequences of present changes in the character of the consumption of inhabitants.

Analysis of legal aspects of the risk in business.

Philosophical aspects of management.

In compliance with the research plan and its item "Development of principles of the environmental philosophy (especially ethics) with regard to the specificities of engineering and technological activities in the field of chemical and food industry" the analysis of genesis and the development of views on the relationship of man of nature in the European cultural traditions was completed at the second stage of the project. The matter in question were developmental changes in the value intentions of the relationship of man of nature in the Renaissance, Reformation and modern-age period. The Renaissance and Reformation had prepared a ground for radical changes in the relationship of man to nature in the modern-time period. The Renaissance justified transformation interventions of the active creative man (homo faber) into the natural environment while the Reformation found the reason for the above interventions, i.e. the economic profit. The modern utilitarianism legitimized man's mastering the nature considering it as a source of the economic growth and an object of the human pragmatic-utilitarian manipulation. In the scientifically and technocratically oriented modern theories the nature appears as a dead sum of sources utilizable by man freely and without limitations. These conceptions have shown the society's developmental trend aimed at the profit and government, which is nowadays from the environmental aspect perspective dangerous because it leads to the subsequent global environmental crisis. Finally, the initial manifestation of criticism of the society's modern developmental trend was of our concern.

Within this item, also the critical analysis of some solutions for proposed strategies of the humanization of nature, particularly for post-modern conceptions based on the so-called non-dualistic and non-anthropocentric approach to the nature was carried out and the appropriate attention was paid to the analysis of some principles of the engineer's environmental and social responsibility. As for the next item of the research plan concerned with "The elaboration of principles of the business ethics with regard to the specificities of managerial and business activities in the chemical and food-industry field", the study of changes in the character of the consumption of inhabitants and the social and psychological as well as political and environmental connections were an object of the project solutions. In agreement with the item of the research plan involving "The elaboration of principles of the commercial and financial legislation in the field of the chemical and food-processing industry in the Slovak Republic with respect to the approximation of the Slovak law to the legal system of the European Union" the analysis of legal aspects of the risk in business in the Slovak Republic was accomplished. Within the item of the research plan related to the "Analysis of the philosophical and social aspects of macroeconomic theories, principles, opinions, solutions and perspectives" the philosophical principles of the management as a key discipline of the economic management were developed.

## **V. COOPERATION**

### **A. Cooperation in Slovakia**

Economic University, Bratislava – Department of Marketing

Technical University, Zvolen – Department of Firm's Economy

University of Transport and Communication, Žilina – Faculty of Management

Technical University, Košice

Philosophical Institute of the Slovak Academy of Sciences, Bratislava

Slovak Philosophical Association, Bratislava

Slovak Association for Purchasing and Logistics, Bratislava

**B. International Cooperation**

Technical University, Vienna, Austria  
 University of Chemistry and Technology, Prague, Czech Republic  
 Economic University, Prague, Czech Republic  
 Private College of Economic Studies, Praha  
 Masaryk University, Brno, Czech Republic  
 Technical University, Ostrava, Czech Republic  
 University of Pardubice, Czech Republic  
 Technical University, Darmstadt, FRG  
 St. Thomas University, Minnesota, U.S.A.

**C. Visitors from Abroad**

October 24: Dr. Iveta Merlinová, Milano, Italy  
 October 11: Assoc. Prof. Ivan Gross, PhD. University of Chemistry and Technology, Prague, Czech Republic  
 October 31: Prof. Eduard Stehlík, PhD., Economic University, Prague, Czech Republic  
 November 8: Assoc. Prof. Hana Lošťáková, PhD., University of Pardubice

**VI. THESES AND DISSERTATIONS****A. Graduate Theses (MS Degree)**

|                          |   |
|--------------------------|---|
| Barami S.:               | Mission of the state budget in the Slovak Republic (Š. György)  |
| Bc. Borosová Z.:         | Position of the joint-stock company in economics of the Slovak Republic (Š. György)                                 |
| Brinza M.:               | Advertising as a key element in the communication mix (D. Špirko)   |
| Čontošová S.:            | The health insurance and health care budget and financing in conditions of VZP Dôvera (D. Baran)                    |
| Dojčanská E.:            | Pricing in conditions of the B+Business centre, Ltd. (J. Kajanová)  |
| Fonóková S.:             | Management and development of human resources in Istrochem, Inc. (P. Herzka)  |
| Ing. Korytár P.:         | Application of controlling of the working capital in a small- and medium-size level of enterprises (D. Baran)       |
| Kováč D.:                | Analysis of job positions and the formation of profesiograms in the human resource management of a firm (P. Herzka) |
| Liptáková A.:            | Internet and the possibilities of its employment (A. Ďurkovičová)   |
| Majtnerová A.:           | The capital market position in the financial market system in the Slovak Republic (D. Baran)                        |
| Neczliová (Drozdová) L.: | Advertising and planning of media within the company's marketing activities (D. Špirko)                             |
| Polčičová B.:            | Motivation in managing people in a large company (P. Herzka)  |
| Reiff M.:                | Prospects of the Slovak capital market in the international context (D. Baran)                                      |
| Roháčková L.:            | Marketing strategies in Datalock, Inc. (M. Jozefček)  |
| Rohošková L.:            | Functions and possibilities of the internet audit in accounting (D. Heseck)   |
| Sajanová Z.:             | Assessment of the economic effectiveness of investment in the Slovak Republic (M. Zatrochová)                       |
| Bc. Svítková M.:         | Financial policy in Slovnaft, Inc. (M. Šostrneková)   |
| Šeboková M.:             | Accounting as an information base in the financial management (D. Heseck)   |
| Trokanová M.:            | Marketing analysis of the market segment of rubber chemicals in Istrochem, Inc. (M. Zatrochová)                     |
| Václavíková K.:          | Leasing as a possibility of the company's financing (P. Velický)  |
| Vallušová B.:            | Accounting of costs and revenues and its exploitation in the decision-making process of a firm (J. Kajanová)        |

**VII. PUBLICATIONS****A. Journals**

- [1] Baran D.: Problémy vymožiteľnosti práva v transformujúcich sa ekonomikách. Problems of the enforcement by law in transforming economics (in Slovak). *Ekonomie a Management* 1, 49-51 (2001). ISSN 1212-3606
- [2] Baran, D.: Marketing of the territory in conditions of the Slovak Republic. *Ekonomie a Management* 3, 53-56 (2001). ISSN 1212-3606
- [3] Baran, D.: Human resource marketing and the firm's sphere. *J. of Human Resource Management* 1-2, 15-30 (2001). ISSN 1335-3888
- [4] Herzka, P.: Aspects of the corporate culture in a chemical enterprise. *J. of Human Resource Management* 2, 10-21 (2000). ISSN 1335-3888
- [5] Špirko, D.: Kresadlové zbrane radu M 1798 "Unterberger". Pechočná puška M 1798 a jej obmeny. Historicko-technická štúdia. Flintlock Firearms of the M 1798 "Unterberger" system. The musket of the M 1798 system and its variants. Historical-technical study (in Slovak). *Guns, Shooters and Hunters* 2, 7-8, 40-42 (2001). ISSN 1335-5740

- [6] Špirko, D.: Kresadlové zbrane radu M 1798 "Unterberger" II. Jazdecké zbrane radu M 1798 a ich obmeny. Ručné strelné zbrane pre jágrov a ostrostrelcov. Ručné strelné zbrane pre osobitné účely a osobitné jednotky. Historicko-technická štúdia. Flintlock Firearms of the M 1798 "Unterberger" system II. Cavalry guns of the M 1798 system and their variants. Hand guns for jaegers and sharpshooters. Hand guns for special purposes and special forces. Historical-technical study (in Slovak). Guns, Shooters and Hunters 2, 9, 18-20 (2001). ISSN 1335-5740

#### **B. Conferences with Proceedings (\*international conferences)**

- [1] Baran, D.: Aplikácia controllingu pracovného kapitálu v podmienkach malých a stredných podnikov. Application of controlling of the working capital in conditions of the small- and medium-size enterprises (in Slovak). Scientific Conference, Senec, Economic University in Bratislava, 17-18 May 2001, p. 7-10. ISBN 80-225-1426-8
- [2] Baran, D.: The system of taxation in the Slovak Republic viewed by an enterpriser. International Conference, VSB Ostrava, 11-12 September, 2001, p. 32-36. ISBN 80-7078-923-9
- [3] Baran, D.: Uplatnenie metód kalkulovania nákladov prostredníctvom aktivít. Application of the methods of costing through activities (in Slovak). In: Proceedings of the 1-st International Conference on "New Trends in the Management of Enterprises". Faculty of Chemical and Food Technology of STU in Bratislava, Senec, 18-19 September 2001, p. 22-25. ISBN 80-227-1612-X
- [4] Baran, D.: Communication in the international marketing mix. In: Proceedings of the Scientific Conference on the Global Business and Economic Development. Faculty of Management of the Comenius University in Bratislava, 7-9 November 2001, published on CD
- [5] Baran, D.: Dôsledky globalizácie na rozvoj malých a stredných podnikov v Slovenskej republike. Consequences of globalization on the development of small- and medium-size enterprises in the Slovak Republic (in Slovak). International Conference, ZU Žilina, 13 November 2001, p. 11-14. ISBN 80-7100-897-4
- [6] Ďurkovičová, A.: Marketingové stratégie uplatňované v strednej a východnej Európe. Marketing strategies applied in Central and Eastern Europe (in Slovak). In: Proceedings of the International Workshop on "the Instruction of Marketing Research in the Context with the Up-to-Date Marketing Theory and Practice. Economic University, Faculty of Commerce, Bratislava, February 2001. p. 8-12. ISBN 80-225-1412-8
- [7] Ďurkovičová, A.: Marketing a internet. Marketing and internet (in Slovak). In: Proceedings of the 1-st International Conference on "New Trends in the Management of Enterprises". Faculty of Chemical and Food Technology of STU in Bratislava, Senec, 18-19 September 2001, p. 37-40. ISBN 80-227-1612-X
- [8] György, Š.: Niektoré otázky dobrých mravov v podnikaní a problémy ekonomickej kriminality. Some questions of good manners in business and problems of the economic criminality (in Slovak). In: Proceedings of the International Seminar on "Humanization of the University Education of Policemen". Academy of the Police Force in Bratislava, Bratislava 2001, p. 199-202. ISBN 80-8054-169-8
- [9] György, Š.: Niektoré právne aspekty rizika podnikania. Some legal aspects of the risk in business (in Slovak). In: Proceedings of the 1-st International Conference on "New Trends in the Management of Enterprises". Faculty of Chemical and Food Technology of STU in Bratislava, Senec, 18-19 September 2001, p. 51-53. ISBN 80-227-1612-X
- [10] György, Š.: Niektoré aspekty dobrých mravov v obchodno-právnych vzťahoch. Some aspects of good manners in the commercial-legal relations (in Slovak). In: Proceedings of the International Seminar on the Role of Methodology in the Systematic Recognition of the Slovak Society in 2000. Ekonóm, Bratislava 2001, p.263-266. ISBN 80-225-1387-3
- [11] Herzka, P.: Some facts about human resource management in the selected regions of Slovakia. In: Proceedings of the International Conference on the Global Business and Economic Development. Faculty of Management of the Comenius University in Bratislava, Bratislava 2001, published on CD
- [18] Jozefček, M.: Podpora malého a stredného podnikania na Slovensku. Support to the small and medium enterprising in Slovakia (in Slovak). In: Proceedings of the Scientific Conference on the Business Environment in the Slovak Republic – Present State and Perspectives III. (in Slovak). Economic University, FPM, Bratislava. May 2001, p. 88-89. ISBN 80-225-1426-8
- [19] Jozefček, M.: Podpora malého a stredného podnikania – personálne stratégie. Support to the small and medium enterprising – personnel strategies (in Slovak). In: Proceedings of the 1-st International Conference on "New Trends in the Management of Enterprises". Faculty of Chemical and Food Technology of STU in Bratislava, Senec, 18-19 September 2001, p. 63-64. ISBN 80-227-1612-X
- [20] Kajanová, J.: Účtovníctvo nákladov a výnosov a jeho využitie v rozhodovacích procesoch. Accounting of costs and revenues and its employment in decision-making processes (in Slovak). International Scientific Conference of Postgraduate Students. Mendel Agricultural and Forest University, Brno, Mendel NET 2001, p. 273-276
- [21] Kajanová, J.: Vplyv daňovej politiky na rozvoj podnikateľskej činnosti. Influence of the tax policy on the development of business activity (in Slovak). In: Proceedings of the Scientific Conference on the Business environment in the Slovak Republic – Present State and Perspectives III. Economic University, FPM, Bratislava 2001, p. 90-93. ISBN 80-225-1426-8
- [23] Kajanová, J.: Účtovníctvo ako zdroj informácií. Accounting as a source of information (in Slovak). In: Proceedings of the 1-st International Conference on "New Trends in the Management of Enterprises". Faculty of Chemical and Food Technology of STU in Bratislava, Senec, 18-19 September 2001, p. 65-68. ISBN 80-227-1612-X
- [24] Kajanová, J.: International accounting standards. In: Proceedings of the International Conference on the Global Business and Economic Development. Faculty of Management of the Comenius University in Bratislava, Bratislava 2001, published on CD
- [27] Šostroneková, M.: Cenová stratégia – významný faktor ovplyvňujúci vstup na trhy. Price strategy – an important factor influencing the entry into markets (in Slovak). In: Proceedings of the Scientific Conference on the Business Environment in the Slovak Republic – Present State and Perspectives III. Economic University in Bratislava, Faculty of Management, Senec 17-18 May, 2001, p. 181-184. ISBN 80-225-1426-8
- [28] Šostroneková, M.-Baran, D.: Influence of the competitive environment on pricing. In: Proceedings of the 1-st International Conference on "New Trends in the Management of Enterprises". Faculty of Chemical and Food Technology of STU in Bratislava, Senec, 18-19 September 2001, p. 111-113. ISBN 80-227-1612-X
- [29] Šostroneková, M.: Stav a perspektivy chemických a potravinárskych podnikov. The status and perspectives of chemical and food-processing enterprises (in Slovak). In: Proceedings of the 1-st International Conference on "New Trends in the Management of Enterprises". Faculty of Chemical and Food Technology of STU in Bratislava, Senec, 18-19 September

- 2001, p. 11-15. ISBN 80-227-1612-X
- [30] Šostroneková, M.: Cenová stratégia v chemických podnikoch Slovenskej republiky. Price strategy in chemical enterprises of the Slovak Republic (in Slovak). In: Proceedings of the International Conference on the Global Business and Economic Development. Faculty of Management of the Comenius University in Bratislava, Bratislava 2001, published on CD
- [31] Špirko, D.: Vývojové zmeny hodnoty prírody, kríza tradičného hodnotového konceptu modernej kultúry a koncepcia trvalo udržateľného rozvoja. Evolutionary changes in the value of nature, the crisis of the traditional value concept of modern culture and the conception of the permanently tenable development (in Slovak). In: Proceedings of the International Seminar on the Role of Methodology in the Systematic Recognition of the Slovak Society in 2000. Ekonóm, Bratislava 2001, p. 71-80. ISBN 80-225-1387-3
- [32] Špirko, D.: Nefahké bremeno zodpovednosti za svet. An oppressive burden of the responsibility for the world (in Slovak). In: Proceedings of the 2-nd Slovak Philosophical Congress, IRIS, Bratislava 2001, p. 466-476. ISBN 80-88778-23-9
- [33] Špirko, D.: Zmeny v charaktere spotreby a ich sociálno-psychologické, politické a environmentálne súvislosti. Changes in the character of the consumption and their social-psychological, political and environmental connections (in Slovak). In: Proceedings of the 1-st International Conference on "New Trends in the Management of Enterprises". Faculty of Chemical and Food Technology of STU in Bratislava, Senec, 18-19 September 2001, p. 114-117. ISBN 80-227-1612-X
- [34] Špirko, D.: Nová humanizačná stratégia. The new humanization strategy (in Slovak). In: Proceedings of the Scientific Conference on the Human Environment published on the occasion of the 10<sup>th</sup> anniversary of the Department of humanistic sciences of SvF STU in Bratislava. STU Bratislava 2001, p. 127-134. ISBN 80-227-1619-7
- [35] Velický, P.: Koncepcia univerzálnej skutočnosti. Conception of the universal reality (in Slovak). In: Proceedings of the International Seminar on the Role of Methodology in the Systematic Recognition of the Slovak Society in 2000. Ekonóm, Bratislava 2001, p. 105-113. ISBN 80-225-1387-3
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- [37] Zatrochová, M.: Podnikateľské prostredie na trhu obchodno-komerčných nehnuteľností. Business environment in the market of the trade-commercial real estates (in Slovak). In: Proceedings of the Scientific Conference on the Business Environment in the Slovak Republic-Present State and Perspectives III. FPM. Economic University, Bratislava 2001, p. 214-216. ISBN 80-225-1426-8
- [38] Zatrochová, M.: Vývoj a problémy investovania v chemickom a potravinárskom priemysle na Slovensku. Development and problems of the investment in the chemical and food-processing industry in Slovakia (in Slovak). In: Proceedings of the 1-st International Conference on "New Trends in the Management of Enterprises". Faculty of Chemical and Food Technology of STU in Bratislava, Senec, 18-19 September 2001, p. 131-133. ISBN 80-227-1612-X
- [39] Zatrochová, M.: Problémy rozvoja obchodných nehnuteľností na Slovensku. Problems of the development of commercial real estates in Slovakia (in Slovak). International Scientific Symposium on the Research of Economic and Managerial Processes in the Building Industry and Investment Projects. SVF STU Bratislava, Faculty of Civil Engineering, September 2001, p. 139-141. ISBN 80-227-1583-2

### C. Books and Textbooks

- [1] Baran, D. Analýza hospodárenia podniku. Analysis of the firm's economizing policy (in Slovak). Publishing House of STU, Bratislava, 185 pp. (2001). ISBN 80-227-1517-4
- [2] Baran, D.: Podnikový controlling. Controlling in a firm (in Slovak). Publishing House of STU, Bratislava, 119 pp. (2001). ISBN 80-227-1558-1
- [3] Ďurkovičová, A., Garajová, J.: Marketing. Marketing (in Slovak). Publishing House of STU, Bratislava, 116 pp. (2001) ISBN 80-227-1466-6

## DEPARTMENT OF MATHEMATICS

**Head of Department:**  
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### I. STAFF

#### Full Professors:

Vladimír Kvasnička, PhD, DSc

#### Associate Professors:

Imrich Fabrici, PhD, Anna Kolesárová, PhD, Jiří Pospíchal, PhD, Michal Šabo, PhD, Štefan Varga, PhD

#### Assistant Professors:

Jozef Antoni, PhD, Vladimír Baláž, PhD, Július Bánki, PhD, Štefan Boor, Ivan Garaj, PhD, Viera Grusková, PhD, Eva Hainzlová, Vladimír Haluška, PhD, Ľubomíra Horanská, Milan Jasem, PhD, Eva Rovderová, PhD, Soňa Sladká

### II. TEACHING AND RESEARCH LABORATORIES

#### A. Teaching Laboratories:

Laboratory equipped by personal computers for the Basics of Computer Science

### III. TEACHING

#### A. Undergraduate study

##### 1st semester (autumn)

|                           |         |  |
|---------------------------|---------|--|
| Calculus I.               | (3-3 h) | Baláž, Fabrici, Grusková, Jasem, Kolesárová, Kvasnička, Šabo |
| Basic of Computer Science | (1-2 h) | Antoni, Bánki, Hainzlová, Pospíchal                          |

##### 2nd semester (spring)

|              |         |  |
|--------------|---------|--|
| Calculus II. | (4-4 h) | Baláž, Fabrici, Grusková, Jasem, Kolesárová, Kvasnička, Šabo |
|--------------|---------|--|

##### 7th semester (autumn)

|               |         |                      |
|---------------|---------|----------------------|
| Calculus III. | (2-2 h) | Antoni, Garaj, Varga |
|---------------|---------|----------------------|

#### B. PhD Study

##### 2nd Semester (spring)

|   |       |                  |
|---|-------|------------------|
| Optimisation Methods and Advanced Mathematical Statistics | (2 h) | Kvasnička, Varga |
|---|-------|------------------|

#### C. Extracurricular lectures

|                                    |         |   |
|------------------------------------|---------|---|
| Evolutionary Algorithms            | (2-0 h) | Kvasnička, Pospíchal (see web address <a href="http://math.chtf.stuba.sk/evol/prednaska.htm">http://math.chtf.stuba.sk/evol/prednaska.htm</a> , this lecture is presented for computer-science students of Faculty of Mathematics and Physics, Comenius University) |
| Introduction to Cognitive Sciences | (2-0)   | Kvasnička, Pospíchal (see web address <a href="http://math.chtf.stuba.sk/kog_vedy.htm">http://math.chtf.stuba.sk/kog_vedy.htm</a> , this lecture is presented for students of Comenius University)  |
| Cognitive Systems                  | (2-2)   | Kvasnička (this lecture is presented for students of Technical University in Košice)  |

### IV. CURRENT RESEARCH PROJECTS

#### A. Artificial neural networks (Vladimír Kvasnička)

The core of the project is the study of artificial neural networks, which are able to accept directly a structural information represented by acyclic rooted graphs. Such a generalization of neural networks is very important not only for chemical application of neural networks, where structural formulas are used as an input of molecules, but also for computer science in general, where the processing of a structural information belongs to its basic problems. An architecture of a neural network will be divided into two parts. In the first part the structural formula will be directly numerically processed, and the output will serve as an input for a standard neural network. The adaptation process, which optimizes the parameters of the neural network to achieve such an output of the neural network, that would be as close as possible to the required output, is applied to both parts of the neural network. The method will be tested for various classes of molecular properties and structural formulas. Our further activities are concentrated on

an application of recurrent neural networks as cognitive devices for multi agent simulation calculations of an emergence of coordinated communication between agents. It was demonstrated, that if an analogue of Dawkins' memes is used, then a coordinated communication spontaneously emerges. On the other hand, if Dawkins' memes are ignored, then an emergence of coordinated communication between agents does not emerge.

### **B. Evolutionary algorithms (Jiří Pospíchal)**

various evolutionary optimisation algorithms (genetic algorithms, simulated annealing, evolution strategies and tabu search) and their applications for solution of combinatorial NP-complete problems, graph theory problems and for adaptation of neural networks, as well as for optimisation of highly multimodal and deceptive functions. Theoretical study of fuzzy systems and implementation of a learning procedure of fuzzy neural networks by evolutionary algorithms. Artificial life studies are performed by making use of evolutionary algorithms as simulators of Darwinian evolution. An emergence of cooperation and altruism in multiagent systems is simulated. Artificial chemistry, typogenetics, models of evolution of autoreplicatory molecules and simulations of origin of life, Darwinian evolution on molecular level.

### **C. Theory of fuzzy systems (Anna Kolesárová)**

The main goals of this project are the modeling of vagueness and the inference process from imprecise or vague premises. These topics are very important for knowledge-based systems, especially for fuzzy expert systems and the aggregation of vague data. In the area of approximate reasoning there are studied various types of inference rules dealing with the problem of deduction of conclusions in an imprecise setting. Namely, a compositional rule of inference based on various types of triangular norms (or other approximate operators) is studied. The methods which effectively simplify the computational complexity of an inference process are investigated. Since the aggregation of input data into a single output is a background of many theoretical and practical problems, we study various types of aggregation operators that can be successfully used in many valued logic, in the theory of approximate reasoning and decision making. Main attention is paid to the aggregation operators based on triangular norms to the construction methods of new aggregations operators and to the conditional aggregation of data.

### **D. Estimations of unknown parameters in statistical models of direct and indirect measurements (Štefan Varga)**

Our specific field of interest has been estimations and predictions in regression models. Special regression models are models with unknown variance and covariance components called mixed regression models. Estimability and different types of estimations of these components and their applications are topics of our publishing activities.

### **E. Periodic weekly seminar on fuzzy sets and fuzzy logic (Michal Šabo)**

Organised for staff of Department of Mathematics and students of our Faculty.

### **F. Periodic yearly workshop on cognitive science (Vladimír Kvasnička and Jiří Pospíchal).**

An interdisciplinary approach to artificial intelligence, neuroscience and cognitive science, sponsored by Open Society Foundation.

## **V. COOPERATION**

### **A. Cooperation in Slovakia:**

Department of Mathematics and Descriptive Geometry, Faculty of Civil Engineering, Slovak Technical University, Bratislava  
 Department of Computer Science and Engineering, Faculty of Electrical Engineering and Information Technology, Slovak Technical University, Bratislava  
 Institute of Informatics, Faculty of Mathematics, Physics, and Informatics, Comenius University, Bratislava  
 Department of Cybernetics and Artificial Intelligence, Faculty of Electrical Engineering and Information Technology, Technical University of Košice

### **B. International Cooperation:**

Department of Mathematics, University of Bayreuth  
 Institute of Mathematics, Johannes Kepler University, LINZ, AUSTRIA  
 Computer Chemistry Laboratory, Masaryk University, Brno, Czech Republic  
 Department of Organic Chemistry, University of Pardubice, Czech Republic  
 Faculty of Informatics, Masaryk University, Brno, Czech Republic  
 Dept. of Computer Science, University of Alcalá, Spain  
 Department of Mathematical Methods and Models for Applied Sciences, University of Rome "La Sapienza", Italy

### **C. Membership in Domestic Organisations and Societies**

Slovak Academic Society (Kvasnička)  
 Slovak Artificial Intelligence Society  
 Slovak Society of Mathematicians and Physicists  
 Slovak Computer Science Society  
 Slovak Mathematical Society

### **D. Membership in International Organisations and Societies**

European Mathematical Society  
 The EURO Working Group on Fuzzy Sets  
 European Society for Fuzzy Logic and Technology

### **Visitors from Abroad**

A. Rammer, University of New South Wales, Sydney, Australia, February 12-12, 2001.



## H. Visits of Staff Members to Foreign Institutions

- A. Kolesárová, M. Šabo: 22<sup>nd</sup> Linz Seminar on Fuzzy Set Theory, LINZ 2001, Linz, Austria, February 6-10, 2001  
 A. Kolesárová, M. Šabo: Research stay, Johannes Kepler University Linz, Austria, February 2001, 8 days  
 A. Kolesárová: Research stay, University of Alcalá, Spain, July 2001, 3 days  
 A. Kolesárová: Research stay, Ceepus, Budapest University of Technology and Economics, Hungary, June 2001, 21 days  
 V. Kvasnička, J. Pospíchal: Invited plenary lecture at the conference Multi-Agent Systems and Application, Prague, Czech Republic, July 2-13, 2001  
 V. Kvasnička, J. Pospíchal: Invited plenary lecture at the European Conference on Artificial Life, Prague, Czech Republic, September 10-14, 2001  
 V. Kvasnička, J. Pospíchal: 5<sup>th</sup> International Conference on Neural Networks and Genetic Algorithms, Prague, Czech Republic, April 22-25, 2001  
 V. Baláž, V. Kvasnička, J. Pospíchal, M. Šabo, Š. Varga: 3<sup>rd</sup> Scientific Colloquium, Prague, June 26-28, 2001  
 J. Pospíchal: Conference Mendel 2001, Brno, Czech Republic, June 6-8, 2001  
 Š. Varga: Agriculture University of Athens, PhD lectures, May 2001, 1 week

## VII. PUBLICATIONS

### A. Journals (\*registered in Current Contents)

- [1]\* Kolesárová A.: Collapsed input-based aggregation. *Int. J. of Uncertainty, Fuzziness and Knowledge Based Systems* 9, Vol.2 (2001) 217-228.  
 [2]\* Kolesárová A.: Limit properties of quasi-arithmetic means. *Fuzzy Sets and Systems* 124, No.1(2001) 65-71.  
 [3]\* Kolesárová A., Vívona D.: Entropy of T-sums and T-products of L-R fuzzy numbers. *Kybernetika* 37 (2001) 127-145.  
 [4]\* Kvasnička V., Pospíchal J.: Autoreplicators and hypercycles in typogenetics. *J. Chem. Structure (Theochem)* 547(2001)119-138.  
 [5]\* Kvasnička V.: An evolutionary simulation of modularity emergence of genotype-phenotype mappings. *Neural Network World* 5(1) (2001) 473-491.  
 [6] Rovderová E.: Nonlinear ordinary differential equations in physics (Nelineárne obyčajné diferenciálne rovnice vo fyzike). *Obzory matematiky, fyziky a informatiky*, Vol. 30 No. 1 (2001) 1-7.  
 [7]\* Šabo M., Kolesárová A., Varga Š.: Ret operators generated by triangular norms and copulas. *International Journal of Uncertainty, Fuzziness and Knowledge-Based Systems*. Vol. 9, No. 2 (2001) 169-181.

### B. Conferences (\*international conferences)

- [1]\* Baláž V.: Zeros and Fixed Points of Continuous Functions and the Structure of Function Space  $C(R)$ . *Proceedings of 3rd Scientific Colloquium*, June 26-28, 2001, Inst. Chem. Technol., Prague 2001, ISBN 80-7080-423-8, pp.108-112.  
 [2]\* Calvo T., Kolesárová A., Komorníková M., Mesiar R.\*: A Review of Aggregation Operators. *Univ. of Alcalá, Madrid*, 2001, ISBN 84-8138-448-8.  
 [3]\* Garaj I.: Sequential plan of Poisson distribution (Sekvenčný preberací plán Poissonovho rozdelenia), *Proceedings of Mechanical Engineering 2001*, STU Publishing, 22. November 2001, pp. 670-675  
 [4]\* Kolesárová A\*, Záhonová V. : Parametric evaluation of aggregation operators. *Proc. Int. Conf. Mechanical Engineering 2001*, SJF STU, Bratislava, November 2001, pp. 684—689.  
 [5]\* Kolesárová A\*, Vívona D.: Measure of fuzziness of T-sums and T-products of L-R fuzzy numbers. *Proc. 9th Zittau Fuzzy Colloquium 2001*, Zittau, 2001, pp. 46-54. ISBN 3-9808089-0-4  
 [6]\* Kolesárová A\*: A note on the construction of aggregation operators by Mobius transform. *Proc. Int. Conf. Uncertainty Modelling 2001*, Bratislava, 2001, pp. 174-183.  
 [7]\* Kolesárová A.\*, Mordelová J.: 1-Lipschitz and kernel aggregation operators. *Proceedings AGOP 2001*, Oviedo, Spain, 2001, pp. 71-75.  
 [8]\* Kvasnička V.\*, Pospíchal J.: A study of autoreplicators and hypercycles by typogenetics. In: J. Kelemen, P. Sosik: *Advances in Artificial Life, ECAL 2001*, LNAI 2159, Springer 2001, pp. 37-54.  
 [9]\* Kvasnička V., Pospíchal J.: A Multi-agent Study of Interethnic Cooperation. *Lecture notes in artificial intelligence*, vol. 2086, Springer 2001, pp. 415-435.  
 [10]\* Kvasnička V.: Artificial chemistry - a new metaphor for evolutionary algorithms. *6th Online World Conference on Soft Computing in Industrial Applications (WSC6)*, <http://www.cranfield.ac.uk/wsc6>  
 [11]\* Kvasnička V.: A Simulation of Spiking Neurons by Sigmoid Neurons. In V. Kurkova, N.C. Steele, R. Neruda, M. Karny (eds.): *Artificial Neural Nets and Genetic Algorithms; Proceedings of ICANNGA*, Prague 2001. Springer Verlag, Wien 2001, pp. 31-34.  
 [12]\* Kvasnička V.: Artificial chemistry. *Proceedings of 3rd Scientific Colloquium*, June 26-28, 2001, Inst. Chem. Technol., Prague 2001, ISBN 80-7080-423-8, pp. 118-129.  
 [13]\* Kvasnička V.: Artificial chemistry – a new metaphor for evolutionary algorithms. *Proceedings of MENDEL 2001*, PC-DIR, Brno, ISBN 80-214-1894-X, pp. 91-96.  
 [14] Kvasnička V.: Connectionism and a modularity of mind in cognitive science (Konekcionizmus a modularita mysle v kognitívnych vedách). In *proceedings Cognitive Science IV (KOGNITÍVNE VEDY IV: Mozog a kognícia)*, Slovak society for artificial intelligence, 7. 12. 2001, Bratislava, pp. 79-95.  
 [15] Kvasnička V.: Creativity through the cognitive glasses (Kreativita optikou kognitívnych vied). In J. Kelemen, V. Kvasnička, J. Pospíchal: *Cognition and Artificial Life (Kognice a umělý život)*. FPF SU Opava, 2001, ISBN 80-7248-107-X, pp.153-166, in Slovak.  
 [16]\* Pospíchal J.\*, Kvasnička V.: Multistage Decision Making for a Fuzzy Automaton by Simulated Annealing *6th Online World Conference on Soft Computing in Industrial Applications (WSC6)*, <http://www.cranfield.ac.uk/wsc6>  
 [17]\* Pospíchal J.\*, Kvasnička V.: Sixth European Conference on Artificial Life (ECAL 2001), Prague, Czech Republic, 9–14

- September 2001 (report on conference) BULLETIN OF THE EATCS 72, October 2001, pp. 254 -261
- [18]\* Pospíchal J.: Applications of Evolutionary Algorithms in Chemistry. Proceedings of 3rd Scientific Colloquium, June 26-28.2001, Inst. Chem. Technol., Prague 2001, ISBN 80-7080-423-8, pp.150-159.
- [19]\* Pospíchal J.: Evolutionary optimization algorithms: A survey and new trends. In: Energy and Information in Non-linear Systems" (A. Gottvald, Ed.), Proc. of The 4th Japan-Central Europe Joint Workshop on Energy and Information in Non-linear Systems (Brno, Nov. 10-12, 2000); CSAEM, Brno, 2001, pp. 24-27.
- [20] Pospíchal J.: Modelling of tragedy of the commons (Modelovanie tragédie spoločného). In the proceedings J. Kelemen, V. Kvasnička, J. Pospíchal: Cognition and Artificial Life (Kognície a umělý život). FPF SU Opava, 2001, ISBN 80-7248-107-X, pp.265-276.
- [21]\* Pospíchal J.: Optimization of Expensive Functions by Surrogates Created from Neural Network Ensembles. In V. Kurkova, N.C. Steele, R. Neruda, M. Karny (eds.): Artificial Neural Nets and Genetic Algorithms; Proceedings of ICANNGA, Prague 2001. Springer Verlag, Wien 2001, pp. 51-54.
- [22]\* Pospíchal J.: Tragedy of the commons in transportation networks. Proceedings of MENDEL 2001, PC-DIR, Brno, 2001, ISBN 80-214-1894-X, pp. 97-102.
- [23]\* Rovderová E.: Problem of solitary water waves. The 1st International Conference on Applied Mathematics and Informatics at Universities '2001, pp. 130-133.
- [24]\* Sarkoci P.\*, Šabo M.: Information boundedness principle and relevancy transformation operators. Proc. of the international conference UNCERTAINTY MODELLING '2001, M. Komorníková, R. Mesiar (Eds.), Sept. 24-28, 2001, Bratislava, Slovakia, Fac. Civil. Eng., 2001, pp. 111-121.
- [25] Šabo M.: A quality of fuzzy connectives in an inference process (Kvalita fuzzy spojok v inferenčnom procese). In proceedings of D-posets in a systeme of quantum structures (D-posety v systéme kvantových štruktúr), KM, Fak. PVO, VA Liptovský Mikuláš, 19.-21.10.2001, Kalenik, Liptovský Peter
- [26]\* Šabo M.: On Some Connectives in Many Valued Logic. Proceedings of 3rd Scientific Colloquium, June 26-28.2001, Inst. Chem. Technol., Prague 2001, ISBN 80-7080-423-8, pp.136-139.
- [27]\* Varga Š.: Different types of uncertainty in regression models. Proceedings of 3rd Scientific Colloquium, June 26-28.2001, Inst. Chem. Technol., Prague 2001, ISBN 80-7080-423-8, pp.136-139.
- [28]\* Varga Š.: Statistical method in Biology, Biotechnology and Chemistry. Lectures in the PhD Course on Food Science and Technology. Agriculture University in Athens. May 2001.
- [29]\* Varga Š.: Uncertainty in regression models. Proceedings of PRASTAN 2001. Kočovce, September 2001, 154 - 159.

### C. Books and Textbooks

- [1] J. Kelemen, V. Kvasnička, J. Pospíchal (eds.): Cognition and Artificial Life (Kognície a umělý život). FPF SU Opava, 2001, ISBN 80-7248-107-X, pp.153-166, in Slovak and Czech.

### E. Other publications

Conferences organized by the department:

Cognition and Artificial Life (KOGNÍCIA A UMEĽÝ ŽIVOT), 15.-17. Marc 2001, Smolenice, Slovakia (see web homepage <http://math.chtf.stuba.sk/smolenice/index.htm> ).

Cognitive Science IV (KOGNITÍVNE VEDY IV: Mozog a kognícia), 7. 12. 2001, FCHPT STUBratislava (see web homepage [http://math.chtf.stuba.sk/CogSci\\_2001.htm](http://math.chtf.stuba.sk/CogSci_2001.htm) )

2<sup>nd</sup> Seminar on Fuzzy Set Theory and Quantum Structures. Vyhne, May 18-20, 2001.

## DEPARTMENT OF MILK, FATS AND FOOD HYGIENE

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### I. STAFF

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**Assistant Professors:**

Mária Greifová, PhD; Vladimír Mastihuba, PhD; Stanislav Sekretár, PhD; Jaroslav Zemanovič, PhD;

**Research Fellows:**

Bernadette Hozová, PhD; Ľudovít Kuniak, PhD; Vlasta Kuklišová;

**PhD students:**

Martina Hrčková; Denisa Lauková; Iveta Kukurová; Terézia Machalcová; Ivana Niklová; Helena Kandárová;

**Technical Staff:**

Vilma Grmanová; Anna Horvátová; Edita Kovačičová; Eva Nováková; Margita Piatriková;

### II. TEACHING AND RESEARCH LABORATORIES

Laboratory of Milk Chemistry and Technology  
Laboratory of Fat Chemistry and Technology  
Laboratory of Food Microbiology  
Laboratory of Cosmetology  
Laboratory of Applied Biotechnology

### III. TEACHING

#### A. Undergraduate Study

**1st semester (autumn)**

|                             |         |          |
|-----------------------------|---------|----------|
| Laboratory Practice Biology | (0-1 h) | Augustín |
|-----------------------------|---------|----------|

**5th semester (autumn)**

|  |         |          |
|--|---------|----------|
| Fundamentals of Hygiene and Sanitation | (1-1 h) | Hojerová |
|--|---------|----------|

**6th semester (spring)**

|                                   |         |                      |
|-----------------------------------|---------|----------------------|
| Cosmetic and Household Chemistry  | (1-1 h) | Hojerová             |
| Packaging and Packaging Materials | (1-1 h) | Sekretár             |
| Fats Chemistry and oleochemistry  | (1-1 h) | Schmidt, Sekretár    |
| Semestral Project                 | (0-4 h) | all Department Staff |

**7th semester (spring)**

|   |         |                              |
|---|---------|------------------------------|
| Dairy Chemistry and Technology I.                     | (2-0 h) | Greifová                     |
| Laboratory Practice Dairy Chemistry and Technology I. | (0-3 h) | Greifová, Mastihuba          |
| Laboratory Practice Special Food Analysis             | (2-2 h) | Augustín, Hojerová, Sekretár |
| Food Microbiology                                     | (2-0 h) | Valík                        |
| Laboratory Practice Food Microbiology                 | (0-4 h) | Valík, Frank, Hozová         |
| Food Unit Operations                                  | (2-2 h) | Schmidt                      |
| Special Practice Food Unit Operations                 | (0-2 h) | Schmidt                      |
| Semestral Project                                     | (0-4 h) | all Department Staff         |

**8th semester (spring)**

|  |         |  |
|--|---------|--|
| Laboratory Practice Dairy Chemistry and Technology           | (0-3 h) | Greifová, Mastihuba                    |
| Fats, Detergents and Cosmetics                               | (4-0 h) | Schmidt, Sekretár, Hojerová, Zemanovič |
| Laboratory Practice Fats, Detergents and Cosmetics           | (0-3 h) | Schmidt, Sekretár, Hojerová, Zemanovič |
| Microbiology of Milk, Fats and Cosmetics                     | (2-0 h) | Valík                                  |
| Laboratory Practice Microbiology of Milk, Fats and Cosmetics | (0-2 h) | Valík, Kuklišová                       |

**9th semester (autumn)**

|   |         |                    |
|---|---------|--------------------|
| Special Food Microbiology                     | (2-0 h) | Valík              |
| Laboratory Practice Special Food Microbiology | (0-2 h) | Valík              |
| Food Ecohygiene                               | (2-0 h) | Frank              |
| Laboratory Practice Food Ecohygiene           | (0-2 h) | Augustín           |
| Special Dairy and Fat Technologies            | (2-0 h) | Schmidt, Mastihuba |
| Laboratory exercise Special Dairy and         |         |                    |

|   |          |  |
|---|----------|--|
| Fat Technologies                                    | (0-4 h)  | Schmidt, Greifová, Sekretár, Mastihuba |
| Side effluents in Food Industry                     | (2-0 h)  | Augustín                               |
| Laboratory Practice Side Effluents in Food Industry | (0-2 h)  | Augustín                               |
| <b>10th semester (spring)</b>                       |          |  |
| Diploma Project                                     | (0-27 h) | all Department Staff                   |
| <b>B. PhD Study</b>                                 |          |  |

#### IV. CURRENT RESEARCH PROJECTS

##### A. Rapid, specific detection of *Listeria monocytogenes* by antibody-based techniques and on line sensor technology; development of improved control of food safety for industry and the consumer (Katarína Horáková)

Food as a vehicle of infection for *Listeria monocytogenes* was not recognised until 1980s. Prior to this the disease, which can cause central nervous system infection and septicemia, was either from an unknown source or was known to be transmitted directly from an animal reservoir or via hospital cross-infection. At particular risk are compromised individuals such as pregnant women and those with underlying disease. The overall objective of the project is to develop rapid, specific test methods for the detection of *Listeria* in foods, with the aim of introducing appropriate quality control into food production processes of the CCE partners. The method will be used both to assess the quality of raw material and the final food product, including where possible on line sensor technology. Partial objectives: to raise novel antibodies; optimise the laboratory technology; validation of the method; to introduce the method for routine detection; to disseminate the results.

Improving of the functional and biological values of foods and cosmetic products.

##### B. Stabilisation of foods containing fats by application of new types of natural antioxidants (Štefan Schmidt)

Minimisation of the *trans*-isomers fatty acids' formation during the partial hydrogenation of vegetable oils. Optimisation of the conditions during the transesterification of triacylglycerols as alternative to the hydrogenation. Development of the predictive microbiology by the using of computer's technique and the mathematical simulation of the relations between micro-organisms and foods. Investigation of the response of micro-organisms to the factors of the external and internal background with the aim to minimise their growth or reproduction. Increasing of the functional and biological properties of foods by the enzymatic hydrolysis of the proteins. Application of the stabilisers to the improvement of the stability of the physical and chemical properties of the cosmetic and food products at the required microbiological safety.

##### C. Improvement of nutrition and sensory quality of foods via optimising of physico-chemical and biological factors (Vladimír Frank)

The project analyses factors, which affect the selected technically relevant microorganisms, i.e. those microbes causing fermentation, spoiling and/or health risks of foods. Application of isolation and separation methods for determination of volatile compounds in investigated foods and sensory profiling of flavour alterations initiated by chemical and microbial changes of food are under intensive search as well. Other branch of project deals with improvement of technical properties of fats via randomization process, which concurrently saves the biological value of fat products considering, that essential fatty acids content remains unchanged after the process.

#### V. COOPERATION

##### A. Cooperation in Slovakia

Central Laboratory Milex - Progres, a.s., Bratislava  
 Dairy Plant Levice  
 De Miclén, a.s, Levice  
 Dimenzia, s.r.o., Kežmarok  
 Institute of Dairy Research, Žilina  
 Institute of Human Nutrition, Bratislava  
 Institute of Preventive and Clinical Medicine, Bratislava  
 Milex, Nové Mesto nad Váhom  
 National Institute of Public Health, Bratislava  
 Nuclear Powerplant Jaslovské Bohunice  
 Palma - Henkel, a.s., Nové Mesto nad Váhom  
 Palma - Tumys, a.s., Bratislava  
 PHARMASUN, Bratislava  
 Rajo, a.s. Bratislava  
 Ress, s.r.o., Senica  
 Slovak Academy of Sciences, Institute of Chemistry, Bratislava  
 Slovak Academy of Sciences, Institute of Molecular Biology, Bratislava  
 Slovak Academy of Sciences, Institute of Pharmacology, Bratislava

##### B. International Cooperation:

Aluso sro, Prague, Czech Republic  
 - Development of cosmetic products  
 BBSRC Institute of Food Research, Norwich, Great Britain  
 - Development of improved control of food safety for industry  
 - Support for database of predictive microbiology.

- BRDC (Biotechnology Research and Development Corporation) Peoria, IL, USA  
 - Enzymatic modification of natural polymers
- Dublin City University, Biomedical and Environmental Sensor Technology Centre, Dublin, Ireland  
 - Development of improved control of food safety for industry
- Institute of Chemical Technology, Department of Biochemistry and Microbiology, Prague, Czech Republic  
 - Development of improved control of food safety for industry
- Institute of Chemical Technology, Department of Dairy and Fat Technology, Prague, Czech Republic  
 - Education of dairy and fat technology  
 - Natural antioxidants
- Johnson Matthey, Prague, Czech Republic & Johnson Matthey, Royston, UK  
 - Toxicity and antimicrobial efficacy study of cosmetic preservatives
- Gimex, sro, Zlín, Czech Republic  
 - Toxicity and antimicrobial efficacy study of cosmetic preservatives
- Gimex, sro, Zlín, Czech Republic  
 - Household Chemistry
- Milcom-Dairy Research Institute, Prague  
 - Development of improved control of food safety for industry
- NCAUR (National Center for Agricultural Utilization Research), ARS, USDA, Peoria, IL, USA  
 - Enzymatic modification of natural polymers
- Technical University Vienna, Department of Biotechnology, Austria  
 - Proteolytic Enzymes of *Brevibacterium linens*
- Food and Agriculture Organization of the United Nations (FAO)  
 - Consultations on food microbiology

### C. Membership in Domestic Organizations and Societies:

- Commission for Technical Standards no 79 (Cosmetics) of Slovak Institute for Technical Standards (J. Hojerová)
- Slovak Society of Cosmetology (J. Hojerová)
- Editorial board of Bulletin of Food Research (Š. Schmidt)
- Expert of the Slovak National Accreditation Service – Technical Commission TVA-L4 (B. Hozová)
- Incheba, Joint Stock Company - Technical Committee for Cosmetics (J. Hojerová)
- Members of Committee of the Slovak Chemical Society (Š. Schmidt)
- Member of Committee of the Food Section SCHS (B. Hozová, Š. Schmidt, J. Zemanovič)
- Slovak Academy of Agriculture (V. Palo)
- Science - Technical Society (B. Hozová)
- Slovak Chemical Society (V. Frank, M. Greifová, Ľ. Kuniak, V. Mastihuba, I. Niklová, V. Palo)
- Slovak National Committee of International Dairy Federation (V. Palo)
- Slovak Gold – Technical Committee for Cosmetics and Household Products (J. Hojerová)
- Slovak Society of Agricultural, Food and Forestry Science (J. Augustín, V. Palo)

### D. Membership in International Organizations and Societies

- Federation of European Chemical Societies, Division of Food Chemistry (Schmidt)
- Editorial board of European Journal of Lipid Science and Technology (Š. Schmidt)
- Czechoslovak Microbiology Society (J. Augustín, M. Greifová, B. Hozová, Ľ. Valík)
- Austrian Chemical Society, Austria (J. Zemanovič)
- International Federation Society of Cosmetic Chemists (IFSCC), USA (J. Hojerová)

### E. Tempus Programme:

### F. International Scientific Programmes:

Copernicus project PL 979012 "Rapid, specific detection of *Listeria monocytogenes* by antibody-based techniques and on-line sensor technology".

### G. Visitors from Abroad:

- |                         |  |
|-------------------------|--|
| Dr. József Baranyi      | Institute of Food Research, UK (1 day)                             |
| Prof. Vladimír Filip    | University of Chemical Technology, Prague (3 days)                 |
| Ludmila Karamonová MSc. | Institute of Chemical Technology, Prague, Czech Republic (4 weeks) |
| Dr. Petr Roubal         | Milcom-Dairy Research Institute, Prague (2 weeks)                  |
| Prof. Karl Bayer        | University of Agriculture, Vienna, Austria (1 day)                 |
| Mgr. Marek Szoltysik    | University of Agriculture, Wrocław, Poland (1 day)                 |

### Visits of Staff Members and PhD Students to Foreign Institutions:

- |                               |  |
|-------------------------------|--|
| Mária Greifová                | Institute of Chemical Technology, Prague, Czech Republic (2 weeks)   |
| Jarmila Hojerová              | Herbacos – Bofarma sro, Pardubice, Czech Republic (3 days)           |
| Helena Kandárová              | National Institute of Public Health, Prague, Czech Republic (2 days) |
| Vladimír Mastihuba            | Institute of Chemical Technology, Prague, Czech Republic (1 weeks)   |
| Ľubomír Valík, Denisa Lauková | University of Chemical Technology, Prague (2 days)                   |
| Ľubomír Valík                 | National Nutrition Centre, Vilnius, Lithuania (2 weeks)              |

## VI. THESES AND DISSERTATIONS

### A. Graduate Theses (MS Degree) for state examinations after five years of study (supervisors are written in brackets):

|                                |  |
|--------------------------------|--|
| Boráková – Králiková Miroslava | Effect of prooxidative factors on quality of vegetable oils (Š. Schmidt)   |
| Garajová Elena                 | Use of hydrolases in derivatisation of saccharides (V. Mastihuba)  |
| Halabuková Adriana             | Dynamics of microbiological properties of <i>Agaricus bisporus</i> (V. Frank)  |
| Hartiníková Henrieta           | Use of rosemary in stabilisation of fats (S. Sekretár)   |
| Husárová Lenka                 | Hydrophobic modifications of proteins (V. Mastihuba)   |
| Kandárová Helena               | Actual problems in evaluation of stability of UV filters in cosmetics (J. Hojerová)  |
| Kohútová Monika                | Validation of analytical methods for detection of UV filters in cosmetics (J. Hojerová)  |
| Kuzmová Daniela                | Study of growth dynamics of selected contaminants in raw milk and dairy products in region of Eastern Slovakia (J. Augustín)   |
| Laššová Lenka                  | Analysis of growth of yeasts depending on control of media pH temperature (L. Valík)   |
| Melišová Denisa                | Effect of external conditions on the growth and production of amines by <i>Enterococcus faecium</i> (M. Greifová)  |
| Michalovičová Zuzana           | Microbiological control of yoghurt production (L. Valík)   |
| Mrózová Zuzana                 | Dairy related decarboxylases – assay and employment (V. Mastihuba)   |
| Rušňáková Monika               | Proteolysis of food proteins by selected proteases (M. Hrkčková)   |
| Šutariková Katarína            | Chemical and microbial indicators of quality of bryndza cheese (M. Greifová)   |
| Švaňová Ľubica                 | Production of polygalacturonidase by microorganisms ( <i>Candida boidinii</i> and <i>Cryptococcus laurentii</i> ) in physiological and stress conditions (J. Augustín) |
| Turicová – Zajíčková Renáta    | Relation of hygienic and sensoric quality of croissants to external (sorbic acid) and internal (aw) conditions of storage (B. Hozová).                                 |
| Vrbovská Lucia                 | Characterisation of extracts from evening primrose according to their antioxidant activity (I. Niklová)  |
| Zajacová Lucia                 | Effect of additives on the oxidation stability of fats during their microwave (S. Sekretár)  |
| Žemberová Jaroslava            | Microbiological properties of selected frozen foods (V. Frank)   |

### B. Dissertations (PhD):

### C. Dissertations (DSc):

### D. Habilitation Theses:

## VII. PUBLICATIONS

### A. Journals (\*registered in Current Contents)

- [1]\* Buchinger W., Tomaschová J., Zemanovič J., Hampel W. A.: Autodegradation of the extracellular proteases of *Brevibacterium linens* ATCC 9172. *Food Chemistry* 74, 61-68, (2001)
- [2] Hojerová J., Jantová S., Hanusová B., Vollek W.: Antimicrobial efficacy of some interesting preservatives for cosmetics. *SÖFW - Journal* 127 (8), 9-15, (2001).
- [3] Hozová B., Kratmüllerová M.: Assay of antibiotic detection limits in cow's milk model samples and comparison of sensitivity of various detection systems (disk diffusion method, Delvotest SP and Penzym S 100). *Czech J. Food Sci.* 19 (4), 125-131, (2001).
- [4] Hozová B., Lenkeyová I.: Interakcie antibiotík - teoretické poznatky a praktické skúsenosti. Interactions of antibiotics – theoretical knowledge and practical experience (in Slovak). *Mliekarstvo*, 32 (2), 38-42, (2001).
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- [10]\* Niklová I., Schmidt Š., Habalová K., Sekretár S.: Effect of evening primrose extracts on oxidative stability of sunflower and rapeseed oils. *Eur. J. Lipid Sci. Technol.* 103 (2001), No. 5, 299-306.
- [11] Sekretár, S.: Spôsoby aktívneho balenia. Methods of active packaging (in Slovak). *Packaging* 5 (1), 6-7, (2001).
- [12]\* Tkáč J., Voštiar I., Šturdík E., Gemeiner P., Mastihuba V., Annus J.: Fructose biosensor based on d-fructose dehydrogenase immobilised on a ferrocene-embedded cellulose acetate membrane. *Analytica Chimica Acta* 439, 39-46, (2001)

- [13] Valík L., Lauková D., Görner F.: Obsah *Bacillus cereus* a celkový počet mikroorganizmov v pasterizovanej smotane. Content of *Bacillus cereus* and total count of microorganisms in pasteurised cream (in Slovak). Bulletin potravinárskeho výskumu, 40 (3), 209-219, (2001)
- [14] Valík L., Piecková E.: Growth modelling of heat resistant fungi: the effect of water activity. International Journal of Food Microbiology, 63 (1-2), 11-17, (2001)
- [15] Valík L.: Svetový deň mlieka na Chemickotechnologickej fakulte STU. The International Day of Milk on Faculty of Chemical Technology, SUT (in Slovak). Mliekarstvo, 32 (2), 7, (2001)

## B. Conferences (\*international conferences)

- [1] Augustín J., Kolarova N.: Produkcia hydroláz polysacharidov u *Rhizopus*. Production of hydrolases of polysaccharides by *Rhizopus* (in Slovak). In: Proceedings from 22nd Congress of the Czechoslovak Society for Microbiology - Health and Microorganisms, Košice 5th-9th September 2001. Slovakia. p. 115 (2001).
- [2] Augustín J.: Izolácia, purifikácia a zdroje prírodných biopolymérnych látok typu alfa -, a beta –glykánov pomocou extrakčných metód. Isolation, purification and sources of natural biopolymer substances like alpha and beta glycans employing extraction methods. In: Zb. Proceedings from LABORALIM 2001, 7.-8.2.2001 Banská Bystrica, 69-73 (2001).
- [3] Augustín J.: Biologicky aktívne látky a ich farmakologické účinky u hľivy ústřicovitej (*Pleurotus ostreatus*). Biologically active substances and their pharmacological activities from oyster mushroom (*Pleurotus ostreatus*) (in Slovak). Proceedings from 22nd Congress of the Czechoslovak Society for Microbiology - Health and Microorganisms, Košice 5th-9th September 2001. Slovakia. p. 113 (2001).
- [4] Augustín J., Hudecová D.: Produkcia hydroláz polysacharidov u *Aureobasidium pullulans*. Production of hydrolases of polysaccharides by *Aureobasidium pullulans* (in Slovak). In: Proceedings from 22nd Congress of the Czechoslovak Society for Microbiology - Health and Microorganisms, Košice 5th-9th September 2001. Slovakia. p. 114 (2001).
- [5] Augustín J., Schmidt Š., Frank V.: Odpadové mliekarenské vody ako vedľajšie produkty, vznikajúce pri spracovaní mlieka a mliečnych výrobkov. Dairy wastewaters as side effluents produced in processing of milk and dairy products (in Slovak). In: Proceedings from the 53rd. Congress of Chemical Societies Banská Bystrica, 3. – 6. 9.2001. p. 282-283, J-PO11 (2001).
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- [7] Dodok L., Buchtová V., Hozová B., Staruch L., Burisová A.: Vplyv zlepšujúcich prípravkov na reologické vlastnosti ciest. . Effect of enhancers on rheology of doughs (In Slovak). In: Abstracts of the XXXII. Symposium on new trends of food production and evaluation (in Slovak). 28.-30.5.2001 Skalský Dvůr, 47 (2001).
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- [14] Greifová M., Greif G., Lenkeyová I., Sádecká Ž., Staňková A.: Vplyv obsahu NaCl a pH na rast a produkciu aminov *Enterobacter aerogenes* v GTK bujóne. Effect of NaCl content and pH on growth and amines production by *Enterobacter aerogenes* in GTK broth (in Slovak). In: Proceedings from 22nd Congress of the Czechoslovak Society for Microbiology - Health and Microorganisms, Košice 5th-9th September 2001. Slovakia. p.165 (2001).
- [15] Hojerová J.: Svet mora v kozmetike – surovínová základňa pre bezpečnú kozmetiku? The sea world in cosmetics – rawmaterials for safe cosmetics? (in Slovak). In: Abstracts from the V. Conference World of Beauty 2001. Bratislava 31.5. 2001. Ed. Puls Promotion, Bratislava (2001).
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- [18] Hojerová J.: Bytová chémia a iná spotrebná chémia. Household chemistry and other consumer chemistry. In: Workshop for chemistry teachers from primary and secondary schools in district of Nitra. Nitra 4. 10. 2001.
- [19] Hojerová J., Francisciiová E., Kohútová M., Schmidt Š.: Validácia analytických metód pre dôkaz UV filtrov v kozmetických prostriedkoch. Validation of analytical methods for detection of UV filters in cosmetic agents In: Proceedings from the 53rd. Congress of Chemical Societies Banská Bystrica, 3. – 6. 9.2001. pp. 280-281, (2001).
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- [21]\* Horáková K., Greifová M., Seemannová Z., Gondová B., Wyatt G. M.: A microplate method for monitoring of *Listeria monocytogenes* growth kinetics and the influence on the expression of p60 in selected enrichment media. In: Vth International Conference on Agri-Food Antibodies, Prague 2nd-5th October 2001. Czech Republic. p. 75 (2001).

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- [23] Hozová B., Turicová R., Lenkeyová I.: Technologické, mikrobiologické a senzorické aspekty hodnotenia výrobkov typu croissant. Technological, microbial and sensoric aspects of evaluation of croissant-type products. In: Proceedings from the 53rd. Congress of Chemical Societies Banská Bystrica, 3. – 6. 9.2001. pp.284-285, JP012 (2001).
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- [25] Jírová D., Hojerová J.: Aktuálne požiadavky EÚ na dôkaz bezpečnosti kozmetických surovín. Actual EU requirements for safety proof of cosmetic raw stocks (in Slovak). In: 3. conference "Cosmetics - Health - Beauty", 2001, Bratislava
- [26]\* Karamonová L., Rauch P., Wyatt G. M., Greifová M., Horáková K.: Production of antibodies to *Listeria* virulence proteins and development of an ELISA for *L. monocytogenes*. In: VIth International Conference on Agri-Food Antibodies, Prague 2nd-5th October 2001, Czech Republic, 115 (2001).
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- [33] Lenkeyová I., Greifová M., Staňková A., Sádecká Ž., Greif G.: Vplyv konzervačných látok na rast *Enterobacter aerogenes* a produkciu biogénnych amínov. Effect of preservatives on growth of *Enterobacter aerogenes* and production of biogenic amines (in Slovak). In: Proceedings from LABORALIM 2001, 7.-8.2.2001 Banská Bystrica, 295-304 (2001).
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- [35]\* Mrózová Z., Mastihuba V.: A spectrophotometric assay of microbial lysine decarboxylase. In: 22nd Congress of the Czechoslovak Society for Microbiology - Health and Microorganisms, Košice 5th-9th September 2001. Slovakia. p. 251 (2001).
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- [37] Niklová I., Schmidt Š., Sekretár S.: Extrakty pupalky dvojročnej (*Oenothera biennis* L.) a ich antioxidantná aktivita v rastlinných olejoch. Extracts from evening primrose (*Oenothera biennis* L.) and their antioxidant activity in plant oils (in Slovak). In: Proceedings from XXXIX. International conference on fat technology and analytics, Železná Ruda, 16-18.5.2001, 97-101 (2001).
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- [45]\* Urbančíková M., Greifová M., Seemannová Z., Karasová L., Wyatt G. M., Rauch P., Horáková K.: Fluorescence detection of *Listeria monocytogenes* using new antibodies as well as FITC-phalloidin. In: VIth International Conference on Agri-Food Antibodies, Prague 2nd-5th October 2001. Czech Republic. p. 104 (2001).



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### C. Books and Textbooks

- [1] Augustín J.: Povídaní o čaji. Talks about tea (in Czech). Edition FONTANA, Olomouc, 2001, 204 p.
- [2] Pokorný J., Schmidt Š.: Natural antioxidant functionality during food processing. In: Pokorný J., Yanishlieva A., Gordon M. eds: Antioxidants in food. CRC Press, New York 2001, Woodhead Publ, Cambridge 2001, pp. 331-353.

### D. Patents

## DEPARTMENT OF ORGANIC CHEMISTRY

**Head of the Department:**  
Prof. Ľubor Fišera, PhD, DSc

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### I. STAFF

**Full Professors:**

Ľubor Fišera, PhD, DSc; Michal Uher, PhD, DSc;

**Associate Professors:**

Ľubomír Floch, PhD; Tibor Gracza, PhD, DSc; Štefan Marchalín, PhD; Viktor Milata, PhD; František Považanec, PhD; Štefan Stankovský, PhD; Katarína Špirková, PhD; Ladislav Štibrányi, PhD;

**Assistant Professors:**

Mária Bobošíková, PhD; Dušan Berkeš, PhD; Eva Jedlovská, PhD; Anna Koreňová, PhD; Angelika Lásiková, PhD; Vladimír Ondruš, PhD; Peter Šafař, PhD; Jarmila Štetinová, PhD;

**Research Fellows:**

Matej Babjak; Iva Blanáriková; Miloslava Dandárová, PhD; Katarína Kadlečíková, PhD; Jana Sikoraiová; Fridrich Szemes; Daniel Végh, PhD, DSc; Peter Zálupský, PhD; Jozefína Žúžiová, PhD;

**PhD Students:**

Iva Blanáriková; Katarína Cvpová; Petra Černuchová; Branislav Dugovič; Róbert Fischer; Mohamed Mahmoud Hassan; Katarína Hrnčáriková; Pavol Jakubec; Peter Kapitán; Andrej Kolarovič; Róbert Mandúch;

**Technical Staff:**

Eva Kaisová; Jana Lehká; Lila Livařová; Mária Nemcová; Antón Pavlíček; Mária Somorovská; Eva Tobiašová; Stanislav Tomek; Iva Viskupičová; Kvetta Wiesingerová;

### II. TEACHING AND RESEARCH LABORATORIES

Laboratory practice:

Basic Skills in Organic Chemistry Laboratory I, II.

Organic Synthesis Laboratory Projects I, II

Research laboratories:

Laboratory of Organic Synthesis

Laboratory of Chiral Cycloaddition Reactions

Laboratory of Heterocyclic Chemistry

Laboratory of Stereoselective Synthesis

Laboratory of Applied Organic Synthesis

Laboratory of Natural Compounds

Laboratory of Nuclear Magnetic Resonance Spectroscopy

Laboratory of IR and UV Spectroscopy

Laboratory of Gas Chromatography

### III. TEACHING

#### A. Undergraduate Study

**3rd semester**

Organic Chemistry (2-2h)

Marchalín, Gracza

Organic Chemistry Laboratory (0-4h)

all teachers and research workers

**4th semester**

Organic Chemistry (2-2h)

Fišera, Považanec, Uher

Organic Chemistry Laboratory (0-5h)

all teachers and research workers

**5th semester**

Chemical Information (1-1h)

Uher

**6th semester**

Chemical Specialities (2-2h)

Mravec, Štibrányi

Semestral Project (0-4h)

Fišera, Gracza, Jedlovská, Marchalín

Považanec, Stankovský, Špirková,

Štetinová

**7th semester**

Organometallic Compounds (1-1h)

Ondruš

|   |         |  |
|---|---------|--|
| Mechanisms of Organic Reactions I                               | (3-1h)  | Fišera   |
| Bioorganic Chemistry  | (2-0h)  | Uher   |
| Laboratory Project I  | (0-10h) | Šafař, Ondruš  |
| Organic Chemistry III   | (1-1h)  | Považanec  |
| <b>8th semester</b>   |         |  |
| Organic Synthesis   | (2-1h)  | Floch  |
| Asymmetric Synthesis  | (2-1h)  | Gracza   |
| Stereochemistry   | (0-2h)  | Štibrányi  |
| Spectroscopic Methods in the Control of Technological Processes | (2-2h)  | Milata, Segľa  |
| Laboratory Project II   | (0-6h)  | Šafař, Štibrányi   |
| Training at Industrial Production Floor 1                       | 5 days  | Fišera, Gracza, Považanec, Šafař, Štibrányi, Végh              |
| <b>9th semester</b>   |         |  |
| Mechanisms of Organic Reactions II                              | (1-1h)  | Marchalín  |
| Applied Organic Synthesis                                       | (1-1h)  | Považanec  |
| Chemistry of Heterocyclic Compounds                             | (2-0h)  | Stankovský   |
| Physical Organic Chemistry I                                    | (0-2h)  | Milata   |
| Chemistry of Natural Compounds                                  | (2-0h)  | Berkeš   |
| Laboratory Project  | (0-10h) | Fišera, Gracza, Považanec, Šafař, Štibrányi, Végh              |
| <b>10th semester</b>  |         |  |
| Diploma Seminar   |         | Považanec  |
| Diploma Thesis Project  |         | Berkeš, Fišera, Gracza, Marchalín, Milata, Považanec, Špírková |

## IV. CURRENT RESEARCH PROJECTS

### A. Stereoselective cycloadditions of heterocyclic compounds (Lubor Fišera)

The primary aim of Prof. Fišera's research is devoted to the search of the stereoselective and regioselective cycloaddition reactions of chiral or achiral 1,3-dipoles to achiral or chiral alkenes and heterocyclic compounds possessing an endo- or exocyclic C=C double bond with the subsequent transformations of so prepared adducts to the bioactive iminopolyols,  $\beta$ -amino acids, lactones, lactames as well as to the new heterocyclic compounds, hardly accessible by another way and which can have a potential biological activity (pharmaca, agrochemicals).

In the past several years, considerable success has been achieved in this group in the utilization of heterocyclic compounds as dipolarophile components in the 1,3-dipolar cycloaddition (some 60 papers published in this field). The last papers have been devoted to the stereo- and regioselectivity of nitrile oxide and nitron cycloadditions to heterocyclic derivatives having exo- and endocyclic C=C double bond. The syntheses of chiral dipoles and dipolarophiles from the natural materials such as sugars,  $\alpha$ -aminoacids are included. Finally, the utilization of so prepared adducts as the synthetic equivalents by means of photochemical and reductive transformations are used for the synthesis of products of diverse biological activities.

### B. Synthesis, reactions and biological activity of 2H-2-pyranones and 2H-1-benzopyran-2-ones. (Lubomír Floch)

The title  $\alpha$ -pyrones have found applications in medicine and as agrochemicals. The research project aims at preparation of designed  $\alpha$ -pyrones in order to build them into more complex molecules with expected pesticidal and antiproliferation activity. Novel sulfonyl- $\alpha$ -pyrones built in sulfonylureas have been synthesized, the target molecules having molecular formula  $\alpha$ -pyrone (or benzopyrone)-SO<sub>2</sub>-NH-CO-NH-heterocycle. The testing of biological activity is carried out in cooperation with the Department of Microbiology, Biochemistry, and Biology (Prof. K. Horáková).

### C. Stereoselective reactions in natural product synthesis (Tibor Gracza)

The study of stereoselective reactions and their applications for the syntheses of naturally occurring compounds, or optically pure building blocks, represents the principal research area of Dr. Gracza's group. A new, general approach to optically active anhydroalditols have been developed, using the stereocontrolled palladium(II)-catalyzed oxycarbonylation of enitols as a key step. This strategy have been applied in the total syntheses of some cytotoxic natural dihydroxystyryl lactones like (+)-goniofufurone and its 7-epimer, as well as their enantiomers. Extension of Pd(II)-promoted bicyclization to optically pure unsaturated aminopolyols offered a very potent way to polyhydroxylated saturated nitrogen heterocycles, many of which are glycosidase inhibitors (related to deoxynojirromycin, DMDP, castanospermine, swainsonine).

### D. Stereoselective synthesis of indolizines and indolizidines (Štefan Marchalín)

4-Arylsubstituted 1,4-dihydropyridines are well-known compounds used in the treatment of hypertension and other circulatory disorders. In the area of 1,4-dihydropyridines are investigated the reactions of 4-aryl-2-formyl-1,4-dihydropyridines. The reactions of 2-for-myl-1,4-dihydropyridines with compounds with active methylene group were tested. Simple modifications of reaction condition lead to changing of chemo- and/or regioselectivity of reaction. The simple and new methods of preparation of substituted 3-aminoindolizines, di- and tetrahydroindolizines were discovered. The phenanthroindolizidine alkaloids, i.e., tylophorine and antofine, exhibit a wide range of biological properties including antitumor activity. In spite of the intense progress in the synthesis of phenanthroindolizidine alkaloids especially in their stereospecific synthesis there has been no report about the stereospecific synthesis of heteroanalog of tylophorine. Our approach to alkaloid synthesis using *N*-heteroarylmethyl-5-oxoproline as building blocks allowed us to prepare chiral and racemic hetero[*f*]indolizidines, closely related compounds of tylophorine. The new enantiopure (*S*)-thieno- and furo[*f*]indolizidines were synthesized in four steps from easily available (*S*)-*N*-thienyl(furyl)methyl-5-

oxoprolines.

### **E. Synthesis and spectral properties of fused heterocycles (Viktor Milata)**

In last years rich experience in the synthesis of substituted push - pull ethylenes, which are remarkable for their significantly polarised multiple bond, has been collected. Reactions of various types (hetero)arylamines (substituted anilines, aminobenzimidazoles, aminobenzotriazoles, quinoxalines etc.) with activated alkoxyethylenes (alkoxymethylene derivatives of propanedinitrile, dialkyl propanedioates, 2,4-pentanedione, alkyl 3-oxobutanoates, 3-oxobutanenitrile or alkyl cyanoacetates), structure of products and their synthetic utilisation in thermal cyclisation (Gould - Jacobs reaction) - which produce the nalidixic acid type quinolones, imidazoquinolones, triazoloquinolones, pyrazinoquinolones were studied. Also research on dihydropyridines, glutaric acid derivatives and reactions of 1-hydroxymethylbenzotriazole, 1-hydroxymethylbenzimidazole is being carried out.

### **F. Synthesis of analogues natural products (František Považanec)**

The principal research area of Dr. Považanec concerns the study of preparation and reactions of heterocyclic compounds, the emphasis being on polycyclic heterocyclic compounds with built-in 1,4-diazepine skeleton. Dr. Považanec is interested mainly in the cyclization and cyclocondensation reactions, which are expected to furnish polycyclic heterocycles possessing bioactivity.

Recently, chiral substrates aroused his interest in that they allow one to prepare polycyclic heterocycles carrying one or more chiral centres. The presence and appropriate configuration of chiral centres has been recognized as pivotal factor in influencing the range of bioactivity of the diazepine-type substrates.

### **G. Imidoyl chlorides and imidoyisothiocyanates in the synthesis of new condensed ring's systems (Štefan Stankovský)**

In series of quinazoline compounds was found a new synthetic method on the basis of imidoyl or amidinoyl isothiocyanates that enables to avoid the complicated processes starting from anthranilic acid. The obtained quinazoline-4-thiones were used for the synthesis of fused 1,2,4-triazolo-, dihydroimidazo-, trihydropyrimido-, and tetrazolo-quinazolines. Quinazoline fused benzotriazepines and benzotetrazepines were prepared by the suitable functionalization of quinazoline skeleton.

### **H. Synthesis of fused quinazoline derivatives (Katarína Špírková)**

The research activity of Dr. Špírková concentrates on condensed quinazolines, aiming at preparation of tricyclic, potentially bioactive structures, such as 1,2,4-triazolo[4,3-c] quinazolines, 2*H*-imidazo- and 2,3-dihydropyrimido[1,2-c]quinazolines. The annelation of further rings takes place across the thione bond of 3*H*-quinazoline-4-thiones by cyclisation and cyclocondensation reactions.

The quinazolines are also the cornerstone of research into synthesis and properties of structural analogues of folic acid. The target molecules are both classical and non-classical antifolates, based on the 3*H*-quinazoline-4-thione skeleton.

### **I. Synthesis of nitrogen, phosphorous heterocycles (Ladislav Štibrányi)**

Synthesis of 5- and 6-membered nitrogen heterocycles. Preparation and study of substituted triazacyclotriphosphazenes carrying nitrogen, sulphur, or oxygen-containing heteroaromatic ligands. Study of nucleophilic reactions on the hexachlorotriazacyclotriphosphazene with ligands capable of metal-complexing. Computer modelling of structure and reactivity. Preparation of derivatives substituted by 1,3-dithiane and their transformation into carbonyl derivatives.

### **J. Transformation of $\gamma$ -pyranone derivatives to the analogues of naturally occurring bioactive compounds (Michal Uher)**

Project is geared at the preparation of the derivatives with possible biological activity with the perspective to use in pharmacology, cosmetics, agriculture and food industry.  $\gamma$ -Pyranone derivative 5-hydroxy-2-hydroxymethyl-4*H*-pyran-4-one (kojic acid) serves as main substrate for the transformation multifunctional. Its manufacture by fermentation is patented in Slovakia. Its decomposition leads to non-toxic products that can enter the circulation of biogenic elements in the nature.

### **K. Synthesis of oligomers and polymers, based on novel five-membered heterocycles, aiming at study and utilization of their conductivity and opto-electronic properties (Daniel Végh)**

Basic research in the field of novel five-membered heterocycles their oligomers and polymers. Search for simple, high-yield synthetic routes leading to heterocycles the oligomers of which will serve as model for polyheterocycles. The latter are expected to possess electric, opto-electric and electroluminescent properties, qualifying such materials as optical storage media, antistatic coatings, and electronic membranes for microelectronics. Also, they can be used in designing electrochemical energy sources, for instance as polymeric electrolytes, novel batteries, as well as in optical sensors and biosensors for monitoring the environment. We intend to design such novel compounds, capitalizing on the relationships between structure and physical properties, solubility, polymer workability. Based on theoretical consideration and calculated predictions we synthesized novel 2,3-substituted thieno[3,4]pyrazine and new pentacyclic dipyrido [3,2-a, 2',3'-c]-thieno-[3,4]azine derivatives, systems with lowest bandgap (0,7 eV). In order to study the effect of the substituent on the chemical and physical properties (also electrical conductivity) twelve new 3-(3-thienyl)glutaric acid derivatives were prepared by easy, novel one step procedure in multigram quantities. Homo or hetero oligo- and polymerization of derivatives were achieved by chemical and electrochemical polymerisation.

## **V. COOPERATION**

### **A. Cooperation in Slovakia**

Slovakofarma, Hlohovec

Synkola, Bratislava

Duslo, Šafa

Slovak Academy of Sciences, Bratislava

Institute of Chemical Technology, Bratislava

Institute of Food Research, Bratislava

Tau-Chem, Bratislava

Chemko, Strážske  
 Institute of Drugs Research, Modra  
 Tatra Trade, Prievidza  
 Institute of Preventive Medicines, Bratislava  
 National Center of Onkology, Bratislava  
 Georganics, Bratislava  
 Q-Chem, Bratislava

## B. International Cooperation:

Inst. für Organische Chemie TU Vienna, Austria  
 - The synthesis of heterocyclic compounds, organization of Blue Danube Symposium on Heterocyclic Chemistry.  
 Inst. für Organische Chemie Univ. Stuttgart, Germany  
 - Stereoselective dipolar cycloaddition and oxycarbonylation reactions  
 Inst. für Organische Chemie Univ. Berlin, Germany  
 - Stereoselective reactions of chiral nitrones  
 Inst. de Chimie Moleculaire d'Orsay, France  
 - Resau formation recherche.  
 Institute de Chimie Moleculaire, Orsay, Univ. Paris-Sud, France  
 - NMR study of chiral compounds and cooperation in exchange of students.  
 Lab. de Chimie, Univ. Le Havre, France  
 - The synthesis of condensed heterocyclic compounds.  
 Inst. für Festkörperphysik der Uni Vienna, Austria  
 - New materials for microelectronics.  
 Cambridge University, Cambridge, Great Britain  
 - The synthesis of natural polytetramic compounds.  
 Institute of Organic Chemistry, Univ. Debrecen, Hungary  
 - The synthesis of heterocyclic compounds.  
 Institute of Organic Chemistry, TU Wroclaw, Poland  
 - The synthesis of heterocyclic compounds.  
 Institute of Organic Chemistry, U Warsaw, Poland  
 - The synthesis of heterocyclic compounds.  
 Institute of Organic Chemistry, AU Krakow, Poland  
 - The synthesis of heterocyclic compounds.  
 UNED, Madrid, Spain  
 - The synthesis of heterocyclic compounds, NMR spectroscopy.  
 Univerzita, Pardubice  
 - The synthesis of heterocyclic compounds

## C. Membership in Domestic Organizations and Societies

Slovak Chemical Society (Scientific Committee Member Prof. M. Uher, Scientific Committee Member Dr. V. Milata, Head of Group of Organic Chemistry Prof. Ľ. Fišera and 30 Members)

## D. Membership in International Organizations and Societies

American Chemical Society (Prof. Ľ. Fišera)  
 German Chemical Society (Prof. Ľ. Fišera, Dr. T. Gracza)  
 Czech Chemical Society (Prof. Ľ. Fišera, Dr. T. Gracza, Dr. Š. Marchalín, Dr. V. Milata)

## E. TEMPUS Programme

## F. International Scientific Programmes

## G. Visitors from Abroad

|                      |   |
|----------------------|---|
| Prof. U. Jordis      | T. Univ. Vienna, Austria, April 2001 (1 day)                |
| Prof. M. Kočevár     | Univ. Ljubljana, Slovenia, April 2001 (2 days)              |
| N. Puljic            | IUT Orsay, Univ. Paris-Sud, France, May-June 2001 (60 days) |
| A. Raux              | IUT Orsay, Univ. Paris-Sud, France, May-June 2001 (60 days) |
| Prof. S. Polanc      | Univ. Ljubljana, Slovenia, June 2001 (4 days)               |
| Dr. A. Kos           | MDL, Switzerland, June 2001 (1 day)                         |
| C. Ikonomidi         | Univ. Athen, Greece, June-July, 2001 (42 days)              |
| H. Arp-Nielsen       | Univ. Bronshej, Denmark, June-July, 2001 (42 days)          |
| Prof. F. Sauter      | T. Univ. Vienna, Austria, July 2001 (2 days)                |
| Prof. H. Fröhlich    | T. Univ. Vienna, Austria, July 2001 (2 days)                |
| Prof. G. Hajos       | Academy Budapest, Hungary, July 2001 (2 days)               |
| Prof. B. Stanovnik   | Univ. Ljubljana, Slovenia, July 200y (2 days)               |
| Prof. H.-U. Reissig  | Univ. Berlin, Germany, October 2001 (3 days)                |
| Prof. E. M. Carreira | ETH Zürich, Switzerland, October 2001 (1 day)               |
| Dr. H. Thiele        | Brucker, Bremen, Germany, December 2001 (1 day)             |
| Prof. U. Beifuss     | Univ. Hohenheim, Germany, December 2001 (3 days)            |

## H. Visits of Staff Members and Postgraduate Students to Foreign Institutions

M. Babjak Kutná Hora, ČR, 4 days

|  |   |
|--|---|
| D. Berkeš                              | Kutná Hora, ČR, 4 days  |
| I. Blanáriková                         | Kutná Hora, ČR, 4 days  |
| K. Cvopová                             | Kutná Hora, ČR, 4 days  |
| P. Černuchová                          | Univ. Paris-Sud, Orsay, Francúzko, 90 days                              |
| B. Dugovič                             | Kutná Hora, ČR, 4 days  |
| R. Fischer                             | Praha, ČR, 4 days, Kutná Hora, ČR, 4 days                               |
| L. Fišera                              | Univ. Vienna, Austria, 4 days, Ustroň, Poland, 5 days, Brno, ČR, 2 days |
| T. Gracza                              | Kutná Hora, ČR, 4 days  |
| K. Hrnčáriková                         | Univ. Katowice, Poland, 5 days  |
| E. Jedlovská                           | Kutná Hora, ČR, 4 days  |
| K. Kadlečíková                         | Univ. Le Havre, Francúzko, 180 days                                     |
| A. Kolarovič                           | Degussa, Germany, 180 days  |
| A. Koreňová                            | Katowice, Poland, 5 days  |
| A. Lásiková                            | Kutná Hora, ČR, 4 days  |
| Š. Marchalín                           | Univ. Le Havre, Francúzko, 60 days                                      |
| V. Milata                              | Kutná Hora, ČR, 4 days, Katowice, Poland, 4 days                        |
| Univ. Vienna, Austria, 10 days         |   |
| V. Ondruš                              | Univ. Stuttgart, Germany, 59 days                                       |
| J. Sikoraiová                          | Kutná Hora, ČR, 4 days  |
| K. Špírková                            | Kutná Hora, ČR, 4 days  |
| J. Štetinová                           | Kutná Hora, ČR, 4 days  |
| L. Štibrányi                           | Kutná Hora, ČR, 4 days  |
| M. Uher                                | Univ. Katowice, Poland, 5 days, Univ. Krakow, Poland, 5 days            |
| D. Végh                                | Univ. Vienna, Austria, 3 days, Univ. Győr, 15 days, Hungary,            |
| Univ. Mosonmagyarövar, 3 days, Hungary |   |
| J. Žúžiová                             | Kutná Hora, ČR, 4 days  |

## VI. THESES AND DISSERTATIONS

### A. Graduate Theses (MS Degree) for state examinations after five years of study (supervisors are written in brackets):

|                |   |
|----------------|---|
| Balážová S.:   | $\alpha$ -Amino acids as building blocks in the synthesis of chiral ACE inhibitors (F. Považanec)   |
| Bradáč V.:     | Preparation and utilization of chiral maleinimides (V. Ondruš)  |
| Bučko M.:      | Synthetic utilization of imidoyl and amidinoyl isothiocyanates in the synthesis of benzotriazocines (K. Špírková)                                 |
| Brath H.:      | Synthesis and reactions of chiral furo[f]indolizinediones (Š. Marchalín)  |
| Černuchová P.: | Preparation and spectral properties of condensed quinoxalines (V. Milata)   |
| Drucková A.:   | Utilization of 1,3-dipolar cycloadditions of chiral nitrones in the design of modified nucleosides (L. Fišera)                                    |
| Gubala V.:     | Thienyl substituted derivatives of $\alpha$ -aminobutanoic acid (D. Berkeš)   |
| Jakubec P.:    | Crystallization-induced dynamic resolution (CIDR) and its utilization in preparation of enantiomerically pure $\alpha$ -amino acids (D. Berkeš)   |
| Kapitán P.:    | Stereoselective palladium (II)-catalysed oxycarbonylations of unsaturated polyols. Synthesis of (+)-goniothalesdiol (T. Gracza)                   |
| Mandúch R.:    | Reduction of substituted 4-aryl-2-aminobutanolides. Preparation of enantiomerically pure derivatives of 1-aryl-3-aminobutane-1,4-diol (D. Berkeš) |

### B. Dissertations (PhD):

|              |  |
|--------------|--|
| Szemes F.:   | Synthesis and reactivity of hetero[f]indolizidines (Š. Marchalín)  |
| Gogová A.:   | Syntheses and reactions of $\alpha$ -pyrones (L. Floch)  |
| Kubáň J.:    | Stereoselectivity of Chiral Nitron Cycloadditions (L. Fišera)  |
| Lásiková A.: | Synthesis of new heterocyclic compounds and their oligomers with proposed biological activity as angiotensin II receptor antagonists (D. Végh) |

## VII. PUBLICATIONS

### A. Journals (\* registered in Current Contents)

- [1]\* Bardošová M., Hodge P., Koreňová A., Nakanishi F., Tredgold R. H.: Polymerisation of Langmuir-Blodgett Film. Comparison of two different methods. *Thin Solid Film* 397, 8-11 (2001)
- [2]\* Blanáriková I., Dugovič B., Fišera L., Hametner Ch., Prónayová N.: 1,3-Dipolar cycloadditions of D-erythrose- and D-threose-derived nitrones to maleimides. *ARKIVOC* 2 (Printed ed.), 1091-1103 (2001) ISSN 1424-6376. <http://www.arkat-usa.org/ark/journal/Volume2/Part3/Sauter/FS-133F/FS-133F.pdf>
- [3]\* Blanáriková I., Fišera L., Kopaničáková Z., Salanski P., Jurczak J., Hametner Ch.: Synthesis of chiral amino acid - derived nitrones and 1,3-dipolar cycloadditions with acrylic acid methyl ester. *ARKIVOC* 2001, 2. <http://www.arkat-usa.org/ark/journal/Volume2/Part3/Sauter/FS-133F/FS-133F.pdf>

- [usa.org/ark/journal/Volume2/Part3/Tisler/MT-255B/MT-255B.pdf](http://www.arkat-usa.org/ark/journal/Volume2/Part3/Tisler/MT-255B/MT-255B.pdf)
- [4]\* Bobošíková M., Clegg W., Coles S. J., Dandárová M., Hursthouse M. B., Kiss T., Krutošíková A., Liptaj T., Prónayová N., Ramsden Ch. A.: The oxidative rearrangement of furan-2-carboximidamines: Preparation and properties of 2-acylaminofurans. *J. Chem. Soc. Perkin Trans. 1*, 680-689 (2001)
- [5]\* Boduszek B., Végh D., Koreňová A., Uher M.: Novel heterocyclic aminophosphonic acids derived from furan and thiophene. *Polish J. Chem.* 75, 1271-1275 (2001)
- [6]\* Brtko J., Hudecová D., Bransová-Bobálová J., Novotný L., Eybl V., Melnik M., Uher M.: Kojic acid: A superior source of biologically active compounds (Current Experience). *Biomarkers and Environment* 4, 26-30 (2001)
- [7]\* Čík G., Krajčovič J., Veis P., Végh D., Šeršeň F.: Charakterisation and properties of the Copolymer of dipyrido-[3,2-a;2,3-c]/thien-[3,4-c]azine with 3-dodecylthiophene. *Synthetic Metals* 118, 111-119 (2001)
- [8]\* Fröhlich J., Sauter F., Milata V.: <sup>13</sup>C NMR of thia- or aza-substituted butyric acid derivatives. *Magn. Reson. Chem.* 39, 113-114 (2001)
- [9]\* Hrdlovič P., Krajčovič J., Végh D.: Spectral Characteristics of bithiophenes and terthiophenes linked with heterocyclic unit in solution and polymer matrix. *Journal of Photochem. and Photobiol. A: Chemistry* 144, 73-82 (2001)
- [10]\* Jantová S., Urbančíková M., Maliar T., Mikulášová M., Rauko P., Čipák L., Kubíková J., Stankovský Š., Špirková K.: Biological activity of some 4-anilinoquinazolines: cytotoxic, genotoxic and antiprotease effects, induction of necrosis and changes of actin cytoskeleton. *Neoplasma*, 48, 52-60, 2001.
- [11]\* Kettmann V., Lokaj J., Kratky C., Marchalín Š., Sikoraiová J.: trans-5,6a-Dihydro5-phenylisoindolo[1,2-b]benz[1,3]oxazepin-11-one. *Acta Cryst. E57*, 612-614 (2001)
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## B. Conferences (\*international conferences)

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#### D. Patents

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## DEPARTMENT OF ORGANIC TECHNOLOGY

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**Research Fellows:**

Zuzana Cvengrošová, PhD; Magdaléna Štolcová, PhD; Dana Gašparovičová; Katarína Fulajtárová;

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**Technical Staff:**

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### II. TEACHING AND RESEARCH LABORATORIES

**A. Teaching Laboratories:**

Technological laboratory 1, 2, 3, 4  
Computer seminar room

**B. Research Laboratories:**

Laboratory of catalytic processes  
Laboratory of reactor technique  
Laboratory of spectroscopic methods

### III. TEACHING

**A. Undergraduate study**

1. Introductory courses

**4th semester (spring)**

|                                       |         |                          |
|---------------------------------------|---------|--------------------------|
| Organic Technology and Petrochemistry | (3-1 h) | Hronec, Králik, Kaszonyi |
|---------------------------------------|---------|--------------------------|

**6th semester (spring)**

|                     |         |   |
|---------------------|---------|---|
| Fine Chemicals      | (2-2 h) | Mravec  |
| Semestral Project I | (0-4 h) | Cvengrošová, Kaszonyi, Králik, Mravec, Štolcová, Vojtko |

2. Advanced Courses

**7th semester (autumn)**

|  |         |                                    |
|--|---------|------------------------------------|
| Chemical-Engineering Thermodynamics    | (0-2 h) | Vojtko                             |
| Catalysis                              | (2-0 h) | Hronec                             |
| Engineering Calculations on a Computer | (1-2 h) | Kaszonyi                           |
| Processes of Organic Technology        | (2-1 h) | Králik                             |
| Laboratory Practise I.                 | (0-8)   | Vojtko, Mravec, Krátky, Horniaková |

**8th semester (spring)**

|                                     |         |   |
|-------------------------------------|---------|---|
| Kinetics and Reactors               | (0-2 h) | Kaszonyi  |
| Process Design                      | (2-1 h) | Hronec, Králik  |
| Technology of monomers and polymers | (2-0)   | Vojtko  |
| Special Organic Products            | (2-0 h) | Mravec  |
| Analysis of Complex Organic Systems | (0-2 h) | Štolcová, Cvengrošová                                   |
| Laboratory Practise II.             | (0-7 h) | Cvengrošová, Hronec, Kaszonyi, Králik, Mravec, Štolcová |

**9th semester (autumn)**

|                                  |          |   |
|----------------------------------|----------|---|
| Coating materials                | (2-0)    | Kramár, Lapeš   |
| Manufacturing of Pharmaceuticals | (2-1 h)  | Mravec  |
| Laboratory Practise III.         | (0-14 h) | Cvengrošová, Hronec, Kaszonyi, Králik, Mravec, Štolcová, Vojtko |

**10th semester (spring)**

|                            |         |  |
|----------------------------|---------|--|
| Seminar to Master's Theses | (0-3 h) | Cvengrošová, Hronec, Kaszonyi, Králik, Vojtko, |
|----------------------------|---------|--|

Štolcová

**B. Postgraduate study**

Catalysis

(2-0)

Hronec

**IV. CURRENT RESEARCH PROJECTS****A. Catalysts for industrial applications (Milan Hronec)**

## 1. Synthesis of new inorganic catalysts and their application

Various oxidation processes (a direct synthesis of phenol and aniline from benzene, partial oxidation of methane) in the gas phase were studied. Hydroxyapatite and apatite catalysts were mainly used and positive effect of ammonia on the yield of desired products was registered. Catalytic behaviour was correlated with physical-chemical properties of the prepared catalysts.

## 2. Catalysis over zeolites

A detail study of reaction pathways in the alkylation of polyaromatics over zeolite catalysts was performed. Transalkylation of alkylated biphenyls with cyclohexene, which was used as a solvent, was observed. Experimental optimisation based on a proper reaction system and conditions allowed to maximise the yield of the desired linear alkylated polyaromatics.

## 3. Microporous organic materials

Further relationships among morphology, accessibility and catalytic activity of metal catalysts supported on functional polymers were studied. The developed catalysts were tested in the hydrogenation of olefins, substituted nitroaromatics and water-phase reduction of nitrates.

**V. COOPERATION****A. Cooperation in Slovakia:**

Slovnaft, Bratislava

DUSLO, Šaľa

Biotika, a.s. Slovenská Ľupča

**B. International Cooperation:**

ENSCM, Montpellier, France:

- zeolite catalysts

- physico-chemical characterisation of solid catalysts

Universita di Padova, Italy:

- polymer supported catalysts, characterisation

Italian National Centre of Research, Padova - Legnaro, Italy:

- preparation of organic supports for catalysts

Czech Academy of Science, Prague:

- characterisation of polymeric materials as supports for catalysts

**C. Membership in Domestic Organisations and Societies:**

Editorial Board of Journal: Petroleum and Coal,

(M. Hronec, M. Králik)

Editorial Board of Journal: Vlákna a textil

(Fibers and Textile)

(M. Hronec)

SCHS (Slovak chemical Society)

(Hronec, Kaszonyi, Králik, Mravec)

SPCH (Slovak Society for Industrial Chemistry),

Chairman of the Catalysis Society

(M. Hronec)

**D. Membership in International Organisation and Societies:**

National representative of the European Federation of Catalysis Societies (EFCATS) (M. Hronec)

Member of the European Academy of Sciences and Arts

(M. Hronec)

**F. International Scientific Programmes**

- Project No. 8217: Alkylation of polynuclear aromatics for the selective synthesis of dialkylated monomers, precursors of advanced polymers: activity and selectivity of zeolitic catalysts and computational analysis of the experimental results (D. Mravec):
  - ENSCM-CNRS (UMR 5618), Montpellier, France
  - Institute of Polymers, Slovak Academy of Sciences, Bratislava
  - Department of Organic Technology, Slovak University of technology, Bratislava
- Project No. 33S6: Charakteriesieren und Testen von Katalysatoren (M.Hronec):
  - Insitut fur Physikalische und Theoretische Chemie, TU Wien
  - Department of Organic Technology, Slovak University of Technology, Bratislava
- Optimisation of the catalytic properties of synthetic organic matrices through chromatographic and spectrometric analysis ("ad hoc" project without an official registration number, financed individually by participants involved) (M. Králik):
  - Department of Inorganic, Metallorganic and Analytical Chemistry, University of Padova, Italy
  - Department of Physical Chemistry, University of Padova, Italy
  - Italian National Centre of Research, Padova - Legnaro, Italy
  - Czech Academy of Science, Prague
  - Department of Organic Technology, Slovak University of Technology, Bratislava
  - Period of co-operation: January 1997-December 2001

**G. Visitors from Abroad**

|                                  |   |
|----------------------------------|---|
| Prof. H. Vinek                   | TU Wien, May 17, bilateral project  |
| Prof. B. Corain                  | Univeristy of Padova, May 18 – 20, scientific collaboration                 |
| Dr. J. Joffre                    | ENSC Montpellier, May 28 – June 1, 2001, scientific collaboration (project) |
| Prof. L. Červený                 | VŠCHT Prague, June 6, state exams   |
| Prof. B. Corain                  | University of Padova, July 30 - August 1, scientific collaboration          |
| Dr. P. Moreau                    | ENSC Montpellier, September 10-17, scientific collaboration (project)       |
| Dr. P. Canton                    | University of Venice, November 7-9, scientific collaboration                |
| Prof. H. Vinek, Dr. G. Foltinger | TU Wien, November 14, bilateral project                                     |

**H. Visitits of Staff Members and PhD Students to Foreign Institutes:**

|                                     |  |
|-------------------------------------|--|
| V. Krátky                           | University of Padova, November 2000 – April 2001, NATO scholarship         |
| J. Horniaková                       | ENSC Montpellier, January 2001 – July 2001, NATO scholarship               |
| M. Hronec                           | VŠCHT Pardubice, January 24 – 25, 2001                                     |
| M. Hronec                           | VŠCHT Praha, March 20  |
| M. Báhidský                         | Praha, March 27 - 31, School on catalysis EFCAT                            |
| M. Hronec                           | VŠCHT Pardubice, April 2 - 3   |
| M. Králik                           | Univeristy of Padova, May 1 – 6, collaboration on the project              |
| M. Hronec                           | VŠCHT Praha, June 5 – 6, 16  |
| M. Hronec, A Kaszonyi, M. Báhidský  | TU Wien, July 3, bilateral project   |
| D. Mravec                           | Montpellier, July 8-23, conference IZC 13, bilateral French-Slovak project |
| M. Králik                           | University of Padova, July 26 – 30, collaboration on the project           |
| M. Hronec                           | Limerick, September 1 – 7, conference Europacat V                          |
| M. Hronec                           | Berlin, September 15 – 21, World congress about oxidation processes        |
| M. Báhidský                         | TU Wien, October 10 – 18, bilateral project                                |
| B. Horváth                          | TU Wien, October 12, bilateral project                                     |
| M. Králik                           | ENSCM Montpellier, October 15 – 23, French-Slovak project                  |
| M. Hronec, J. Vojtko                | Rožnov p/R, October 22 – 24, conference APROCHEM                           |
| M. Králik, J. Horniaková, V. Krátky | Praha, November 5 – 6, Symposium on catalysis                              |
| M. Hronec                           | Kecskemet (Hungary), November 8 – 10, invited lecture HAS                  |
| M. Hronec                           | Val. Meziříčí DEZA, November 15 – 16, invited lecture, collaboration       |
| M. Hronec, M. Štolcová, M. Báhidský | TU Wien, December 17, bilateral project                                    |

**VI. THESES AND DISSERTATIONS****A. Graduate Theses (MS Degree) for state examinations after five years of study (supervisors are written in brackets)**

|               |   |
|---------------|---|
| Babálová S.:  | Terc.butylácia toluénu na zeolitových katalyzátoroch. Tert-butylation of toluene over zeolite catalysts (Mravec D.)   |
| Gogová Z.:    | Oxidácia cyklohexylamínu na cyklohexanónoxím v plynnej fáze. Gas phase oxidation of cyclohexylamine to cyclohexanone oxime (Cvengrošová Z.)   |
| Janičková J.: | Štúdium vlastností katalyzátorov oxidačnej dimerizácie amínu. Study the properties of the catalysts for the oxidation dimerization of aniline (Štolcová M.)   |
| Jaško Z.:     | Vplyv UV a IČ žiarenia na oxidáciu cyklohexylamínu. Influence of UV and IR radiation on the oxidation of cyclohexylamine (Kaszoniy A.)  |
| Ješíková I.:  | Katalytická redukcia dusičnanov vo vode na bázičických Pd-Cu katalyzátoroch. Catalytic reduction of nitrates in water over basic Pd-Cu catalysts (Králik M.)  |
| Juhás E.:     | Premena metánu na fosfátových katalyzátoroch. Transformation of methane over phosphate catalysts (Štolcová M.)  |
| Mečárová M.:  | Hydrogenácia chlórinitrobenzénov. Hydrogenation of chloronitrobenzenes (Králik M.)  |
| Michalica P.: | Syntéza pyridínu kondenzačnou reakciou karbonylových zlúčenín, alkoholov a NH <sub>3</sub> . Synthesis of pyridine by condensation reaction of carbonyl compounds, alcohol and NH <sub>3</sub> (Cvengrošová Z.) |
| Oswald E.:    | Aminácia benzénu amoniakom. Amination of benzene by ammonia (Kaszoniy A.)   |
| Radičová G.   | Katalytická redukcia dusičnanov vo vode na slabokyslých Pd-Cu katalyzátoroch. Catalytic reduction of nitrates in water over weak-acid Pd-Cu catalysts (Králik M.)   |

**B. Dissertation (PhD)**

|              |   |
|--------------|---|
| Michvocík M. | Alkylation of polycyclic aromatic hydrocarbons over zeolite catalysts (Mravec D.) |
|--------------|---|

## VII. PUBLICATIONS

### A. Journals (\*registered in Current Contents)

- [1]\* Corain B., Králik M.: Generating of palladium nanoclusters inside functional cross-linked polymer frameworks. *J. Mol. Catal. A: Chemical* 173, 99 - 115 (2001)
- [2]\* Horniaková J., Mravec D., Králik M., Leško J., Graffin P., Moreau P.: Tert-butylation of biphenyl over HY a H-beta zeolites, formation and identification of main and by-products. *Appl. Catal. A: General* 215, 235 - 244 (2001)
- [3]\* Horniaková J., Králik M., Kaszonyi A., Mravec D.: A practical approach to the treatment of adsorption-desorption isotherms, acidity and catalytic behaviour of zeolite catalysts. *Micropor. Mater.* 46, 287 - 298 (2001)
- [4]\* Horniaková J., Mravec D., Moreau P.: Tert-butylation of biphenyl over mordenites. *Catal. Lett.* 75 (3 - 4), 163 - 167 (2001)
- [5]\* Králik M., Biffis A.: Catalysis by metal nanoparticles supported on functional organic polymers. *J. Mol. Catal. A: Chemical* 177, 113 - 138 (2001)
- [6]\* Štolcová M., Kaszonyi A., Hronec M.: Reaction of N-alkyl-2-benzothiazolesulphenamide with acetic anhydride in the presence of acids. I. Technological aspects. *J. Mol. Catal. A: Chemical* 172, 165 - 173 (2001).
- [7]\* Štolcová M., Grošková D., Hronec M.: RP-HPLC for the determination of N-phenylhydroxylamine and related compounds. *Chromatographia* 53, S 456 - S 459 (2001)
- [8]\* Štolcová M., Kaszonyi A., Hronec M., Liptaj T., Staško A., Leško J.: Reaction of N-alkyl-2-benzothiazolesulphenamide with acetic anhydride in the presence of acids. II. Spectral studies. *J. Mol. Catal. A: Chemical* 172, 175 - 186 (2001)
- [9]\* Králik M., Horniaková J., Mravec D., Jorík V., Michvocík M., Moreau P.: Texture of dealuminated mordenite catalysts modified with cerium and catalytic properties in the isopropylation of biphenyl. *Studies in Surface Science and Catalysis* 135, 313 (2001)
- [10]\* Mravec D., Horniaková J., Králik M., Hronec M., Joffre J., Moreau P.: Shape-selective tert-butylation of biphenyl over H.MOR, H - Y and H - BEA zeolites in the liquid phase. *Studies in Surface Science and Catalysis* 135, 280 (2001)
- [11]\* Joffre J., Mravec D., Moreau P.: Computational analysis of the shape-selective isopropylation of biphenyl over large-pore zeolites. *Studies in Surface Science and Catalysis* 135, 264 (2001)
- [12]\* Derco J., Králik M., Kovács A.: Modelling of Nutrient Removal Processes in an Intermittently Aerated Bioreactor. *Chem. Biochem. Eng.* 15(4), 167-174 (2001)
- [13] Králik M., Macho V., Brautbar N., Vachalková A., Mikulec J.: Engine fuels in the 21st century. *Petroleum and Coal* 43 (2), 72 - 79 (2001)
- [14] Derco J., Králik M.: Optimisation of an oil wastewater treatment plant. *Petroleum and Coal* 43 (2), 85 - 88 (2001)
- [15] Derco J., Gulyášová A., Králik M., Mrafková L.: Treatment of an industrial wastewater by ozonation. *Petroleum and Coal* 43 (2), 92 - 97 (2001)
- [16] Mravec D., Horniaková J., Moreau P., Joffre J.: Shape-selective alkylation of biphenyl: Comparison between tert-butylation and isopropylation over different zeolites. *Petroleum and Coal* 43 (2), 107 - 110 (2001)
- [17] Štolcová M., Juhás E., Hronec M.: Partial oxidation of methane over iron - calcium - phosphorus catalysts. *Petroleum and Coal* 43 (2), 111 - 114 (2001)
- [18] Brautbar N., Králik M., Macho V., Mikulec J., Vachalková A.: A continuation of the MTBE story. *Petroleum and Coal* 43 (2), 101 - 106 (2001)

### B. Conferences (\*international conferences)

- [1]\* Liptáková B., Hronec M.: Oxidation of Benzene Over Mixed Calcium-Copper hydroxyapatite Catalysts. XXXIII. Symposium on Catalysis, Prague Nov. 5 - 6. 2001, 2 pp. (Po)
- [2]\* Krátky V., Králik M., Mečárová M., Zalibera L., Hronec M.: Selective hydrogenation of chloronitrobenzenes over palladium supported catalysts. *Europacat V*, 2. - 7. 9. 2001, 13 - P - 14 (Po)
- [3]\* Štolcová M., Hronec M.: Partial oxidation of methane over Ca-Fe-P containing catalysts. 53. zjazd chemických spoločností, Banská Bystrica, 3. - 6. 9. 2001, Zborník príspevkov p. 15 - 16 (Le)
- [4]\* Králik M.: Syntetické funkcionizované organické polyméry ako nosiče pre katalyzátory s dispergovanými kovmi. Synthetic functional polymers as supports for catalysts with dispersed metals. 53. zjazd chemických spoločností, Banská Bystrica, 3. - 6. 9. 2001, Zborník príspevkov p. 17 - 18 (Le)
- [5]\* Kaszonyi A., Hronec M.: Direct amination of benzene by ammonia. 53. zjazd chemických spoločností, Banská Bystrica, 3. - 6. 9. 2001, Zborník príspevkov p. 58 - 59 (Le)
- [6]\* Kaszonyi A., Štolcová M., Hronec M.: Determination and identification of major and minor reaction products of direct amination of benzene. 11th International Symposium, Advances and Applications of Chromatography in Industry, Bratislava, August 27 - 31, 2001, ISSN 1335-8413 (Po)
- [7]\* Macho V., Králik M.: "Sírny" katalytický systém karbonylačnej redukcie a reductívnej karbonylácie aromatických nitrózo- a nitrozlučenín. Sulphur catalytic system of the carbonylative reduction and reductive carbonylation of aromatic nitroso and nitrocompounds. 53. zjazd chemických spoločností, Banská Bystrica, 3. - 6. 9. 2001, Zborník príspevkov s. 29 - 30 (Po)
- [8]\* Štolcová M., Kaszonyi M., Hronec M., Fulajtárová K.: Identification of minor components formed from N-alkyl-2-mercaptobenzothiazole derivatives in an acidic medium. 11th International Symposium Advances and Applications of Chromatography in Industry, Bratislava, August 27 - 31, 2001, ISSN 1335-8413, 2 pp (Po)
- [9]\* Králik M. Catalysis by dispersed metals in the 1st year of the 21st century. 28<sup>th</sup> International Conference SSCHE, Proceedings on CD ROM, Tatranské Matliare (SK), 21 - 25 May, 2001, ISBN 80-227-1533-6, 11 p (Pi.Le)
- [10]\* Králik M., Ješíková I., Radičová G.: Recent results from the catalytic water-phase removal of nitrates over Pd-Cu catalysts supported on basic and mild-acid ionic resins 28<sup>th</sup> International Conference SSCHE, Proceedings on CD ROM, Tatranské Matliare (SK), 21 - 25 May, 2001, ISBN 80-227-1533-6, P115, 6 pp (Po)
- [11]\* Krátky V., Mečárová M., Zalibera L., Králik M.: Effect of a solvent on the selectivity in the hydrogenation of chlorinated nitroaromatics. 28<sup>th</sup> International Conference SSCHE, Proceedings on CD ROM, Tatranské Matliare (SK), 21 - 25 May, 2001, ISBN 80-227-1533-6, P117, 4 pp (Po)
- [12]\* Macho V., Králik M., Cingelová J., Vajdová J., Matej M.: Regeneration and Recycling of polyurethanes by glycolysis. The 6<sup>th</sup>

- International Conference on Theoretical and Experimental Problems of Materials Engineering. ISBN 80-968099-5-4, p. 29 (Le)
- [13]\* Brautbar N., Králik M., Macho V., Mikulec J., Vachálková A.: A continuation of the MTBE story. 40 th International Petroleum Conference, 17. - 19. Sept. 2001, ISSN 1335-888X, L-A-1, 13 pp (Le)
- [14]\* Králik M., Macho V., Brautbar N., Vachálková A., Mikulec J.: New trends in solution of technological and acological problems with dialkyl ethers applied in reformulated gasoline. 40 th International Petroleum Conference, 17. - 19. Sept. 2001, ISSN 1335-888X, L-A-3, 17 pp (Le)
- [15]\* Kaszonyi A., Cvengrošová Z., Hronec M.: Oxidation of cyclohexylamine over polyoxometalates of tungsten. 40 th International Petroleum Conference, 17. - 19. Sept. 2001, ISSN 1335-888X, L-E-4, 9 pp (Le)
- [16]\* Macho V., Králik M., Cingelová J., Kavala M.: Possibilities of one-stage preparation and utilization of epoxy-compounds from dienes. 40 th International Petroleum Conference, 17. - 19. Sept. 2001, ISSN 1335-888X, L-E-5, 10 pp (Le)
- [17]\* Štolcová M., Hronec M., Juhás E.: Partial oxidation of methane over iron - phosphorus catalysts. 40 th International Petroleum Conference, 17. - 19. Sept. 2001, ISSN 1335-888X, L-E-7, 7 pp (Le)
- [18]\* Derco J., Gulyášová A., Králik M., Mrafková L.: Treatment of an industrial wastewater by ozonation. 40 th International Petroleum Conference, 17. - 19. Sept. 2001, ISSN 1335-888X, L-G-4, 12 pp (Le)
- [19]\* Cvengroš J., Cvengrošová Z., Hóka Cs.: Transesterification of vegetable oils to methylesters and determination of conversion by TLC method. 40 th International Petroleum Conference, 17. - 19. Sept. 2001, ISSN 1335-888X, P-D-24, 6 pp (Le)
- [20]\* Mravec D., Horniaková J., Moreau P.: Shape - selective alkylation of biphenyl. 40 th International Petroleum Conference, 17. - 19. Sept. 2001, ISSN 1335-888X, P-E-38, 8 pp (Po)
- [21]\* Derco J., Gulyášová A., Králik M., Mrafková L.: Treatment of an industrial wastewater by ozonation. 40 th International Petroleum Conference, 17. - 19. Sept. 2001, ISSN 1335-888X, L-G-4, 12 pp (Le)
- [22]\* Derco J., Králik M.: Optimization of an oil wastewater treatment plant. 40 th International Petroleum Conference, 17. - 19. Sept. 2001, ISSN 1335-888X, P-G-50, 7 pp (Po)
- [23]\* Krátky V., Králik M., Štolcová M., Zalibera L., Hronec M.: Hydrogenation of chloronitrobenzenes, catalys and solvent effects. XXXIII. Symposium on Catalysis, Prague Nov. 5 - 6. 2001, 2 pp (Le)
- [24]\* Horniaková J., Mravec D., Králik M., Moreau P.: Shape - selective tert-butylation of biphenyl. XXXIII. Symposium on Catalysis, Prague Nov. 5 - 6. 2001, 2 pp (Le)
- [25]\* Biffis A., Ricoveri R., Králik M., Jeřábek K., Corain B.: Highly chemoselective hydrogenation of 2-ethylantraquinone to 2-ethylantrahydroquinone catalyzed by palladium metal dispersed inside very lipophilic functional resins. XXXIII. Symposium on Catalysis, Prague Nov. 5 - 6. 2001, 3 pp (Po)
- [26]\* Gomory J., Králik M.: Selective hydrogenation of pseudoionone to hexahydropseudoionone. XXXIII. Symposium on Catalysis, Prague Nov. 5 - 6. 2001, 2 pp (Po)
- [27] Macho V., Králik M., Cingelová J., Vajdová J.: Hydrogenácia vyšších monokarboxylových a dikarboxylových kyselín na vyššie alkoholy a dioly. Hydrogenation of higher monokarboxylic and dikarboxylic acids to higher acohols and diols. Chemprogres 2001. jún 2001, Púchov, pp 31-32 (Le)
- [28] Macho V., Králik M., Komora L., Cingelová J.: Pokroky v príprave organických medziproduktov: laktónov a alkylaktónov, alkanolov diolov a amidov karboxylových kyselín. Advances in the preparation of intermediates for: lactones, alkylactones, alkanols, diols and amids of carboxylic acids. APROCHEM, Rožnov p/R., ČR, 22. - 24. 10. 2001, Zbomník s. 210 – 213. (Le)
- [29] Vojtko J.: Nové smery využitia pyrolýzy v organickej technológii. New Trends in Exploitation of Pyrolysis in OrganicTechnology. APROCHEM, Rožnov p/R., ČR, 22. - 24. 10. 2001, Zbomník s. 216 – 221 (Le)

### C. Books and Textbooks

- [1] Corain B., Králik M. (Eds.): Catalysis with Supported Palladium Metal at the Turn of the 21<sup>st</sup> Century. Special issue of J. Mol. Catal. A: Chemical 173(1-2) (2001) ISSN 1381-1169. 356 pp
- [2] Corain B., Jerabek K., Králik M. (Eds.): Catalysis inside Functional Synthetic Resins: The issue of Catalysts Accessibility and Stability. Special issue of J. Mol. Catal. A: Chemical 177 (2001) ISSN 1381-1169. 170 pp

### D. Patents

- [1] Kaszonyi A, Bábi J.: Leptacie činidlo na sklo. Etching agent for glass. SK 3084 (3. 12. 2001)
- [2] Macho V., Mravec D., Vojtko J., Králik M., Gattnár O., Varga I., Šnupárek V., Škoda A.: Spôsob výroby kyseliny azelaovej a/alebo kyseliny malónovej a/alebo ich metylesterov. Manufacture of azelaic acid and/or malonic acid and/or their methyl esters. SK 281462 (9. 4. 2001)

### E. Research reports

- [1] Hronec M. et al.: New catalysts for industrial applications. Final report on the SK VEGA project 1/6049/99.

## DEPARTMENT OF PETROLEUM TECHNOLOGY AND PETROCHEMISTRY

**Head of Department:**  
Assoc. Prof. Pavol Daučík, PhD

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### I. STAFF

#### Full Professors:

Martin Bajus, PhD, DSc;

#### Associate Professors:

Pavol Daučík, PhD; Pavol Hudec, PhD; Agáta Smiešková, PhD; Zdenek Židek, PhD;

#### Assistant Professors:

Elena Hájeková, PhD;

#### Research Fellows:

Jozef Ambro; Pavol Kaláb; Beata Liptáková; Peter Michalica

#### PhD Students:

Jozef Ilkovič; Jozef Okuliar; Roman Svitaň; Ľuboš Šabo;

#### Technical Staff:

Adriana Brezová; Marcela Hadvinová; Dagmar Machatová; Marta Olleová; Emil Pribiš; Helena Šuňalová;

### II. TEACHING AND RESEARCH LABORATORIES

Laboratory of Catalysts Characterization

Laboratory of High Pressure Reactors

Laboratory of Gas and Liquid Chromatography

Laboratory of Chemistry and Analysis of Fuels

Laboratory of Pyrolysis

Laboratory of Rheology of Lubricants

Laboratory of Infra-Red Spectroscopy

Laboratory of Natural Gas Conversion

Wiped-film Molecular Evaporator

### III. TEACHING

#### A. Undergraduate study

##### 4th Semester (spring)

|                                       |         |                          |
|---------------------------------------|---------|--------------------------|
| Organic Technology and Petrochemistry | (3-1 h) | Bajus, Smiešková, Daučík |
|---------------------------------------|---------|--------------------------|

##### 7th Semester (autumn)

|                                      |         |                  |
|--------------------------------------|---------|------------------|
| Catalysis                            | (0-1 h) | Hudec            |
| Analysis of Petroleum Products       | (2-0h)  | Daučík           |
| Technology of Crude Oil              | (3-0 h) | Židek, Smiešková |
| Combustion Processes                 | (1-2 h) | Smiešková        |
| Engineering Calculations on Computer | (0-2)   | Ambro            |
| Laboratory exercise 1                | (0-8 h) | Daučík           |

##### 8th Semester (spring)

|   |         |          |
|---|---------|----------|
| Alternative Fuels   | (2-0 h) | Bajus    |
| Catalytic and Thermal Processes<br>in Crude Oil Treatment | (3-0 h) | Židek    |
| Tribology   | (2-0 h) | Hájeková |
| Kinetic and Reactors                                      | (0-2 h) | Hudec    |
| Laboratory exercise II                                    | (0-8 h) | Hudec    |

##### 9th Semester (autumn)

|                                   |          |        |
|-----------------------------------|----------|--------|
| Petrochemistry                    | (3-0 h)  | Bajus  |
| Refinery and Petrochemical Plants | (1-1 h)  | Daučík |
| Laboratory exercise III           | (0-10 h) | Hudec  |

#### B. PhD study

|   |       |       |
|---|-------|-------|
| Technology of Crude Oil                                   | (3 h) | Židek |
| Petrochemistry  | (3 h) | Bajus |
| Catalytic and Thermal Processes in<br>Crude Oil Treatment | (3 h) | Židek |

## IV. CURRENT RESEARCH PROJECTS

### A. New catalysts for industrial applications (Milan Hronec)

In petroleum industry and petrochemistry, still growing applications find a catalytic materials with precisely defined structure and acido-basic properties. Among such suitable catalysts, zeolites and ordered mesoporous materials play role as basic components. The project is oriented to development of knowledge of the role of heterogeneous catalysts in selected refinery and petrochemical processes, to develop the relation between composition, structure and method of the catalysts preparation and their catalytic properties. The research is oriented into following subjects:

1. Characterization of influence of extraframework aluminum on acid and catalytic properties of zeolites USY and steamed ZSM-5 (measured by XRD, IR, TPDA, surface area, pore size distribution, distribution of Broensted and Lewis acid sites and their common induction effect). Influence of the stabilization conditions and method of following acid modification are studied.

2. Study of method of the incorporation and quantity of zinc and it influence on the activity of Zn-ZSM-5 zeolites in aromatization of light hydrocarbons - examination of liquid ion exchange as well as solid state ion exchange, characterization of samples by TPDA, IR and by catalytic tests.

3. Preparation of materials with ordered mesoporous structure as MCM-41. Such materials are potential suitable components of the new generation of FCC, HC and HR catalysts in relation to their wide mesoporous structure with the pore diameter of 4 - 10 nm.

4. Hydrotreating (HDS, HDN) of middle petroleum distillates with the aim to explain the reason of lower color stability of gasoline, kerosene and gas oil from hydrocracking of heavy residues. Studies are carried out in a laboratory pressure reactors using commercial hydrotreating catalysts under conditions used in refineries.

### B. Interactions between composition and properties of fuels, lubricants and heavy oil products (Pavol Daučík)

Oil products quality improvement is a general trend to utilize more effectively the expensive raw material, to prolong the lifetime of machines and equipment where oil products are used. Nowadays it is an obvious requirement to minimize the negative effects of oil products on the environment. Fuels, lubricants and heavy oil products form the major part of products which are actually used in all fields of industry and common consumption. Functional properties are the deciding factors for the product choice in certain use in practice. At comparable qualitative parameters, the economic standpoint is the decisive factor in the choice from the appropriate supply. Then, the price regarding the consumption and qualitative properties is the deciding criteria in the product choice. Nowadays the product choice is expressively influenced by ecological standpoint. It is unequivocal that ecological and economic standpoints contradictory effect on the product choice. Hence, the ecological criteria is influenced only by legislation stated rules. Ecological viewpoint gets then its priority and in some countries the maximum content of aromatics, sulfur and metals are determined by law.

Project is aimed at the interactions between the composition and the properties of oil products and additives. The main target is the evaluation of oxidative stability, reological properties, effects of additives on functional properties of fuels, lubricants and heavy oil products. Project's intention is to utilize correlation between composition and properties of the product to evaluate the quality and the optimal composition of the given product. From the ecological standpoint the determination of aromatic hydrocarbons content, sulfur and metal content is significant, with the goal to evaluate the effect of minimization of the content of these compounds on the functional properties of products.

### C. Thermal and catalytic conversion of petroleum and alternative feedstock to refinery products and petrochemical and theirs biodegradability (Martin Bajus)

Most intermediates and monomers in the petrochemical industry are currently produced starting from alkenes and aromatics as building blocks. Alkenes are obtained mainly by steam cracking (pyrolysis) of hydrocarbon from petroleum and natural gas. The original aim of the research project is based on copyrolysis of high and low molecular hydrocarbons, for example: hexadecane and heptane. Under conditions of copyrolysis of hydrocarbons of paraffinic character to low molecular alkenes and aromatics, there occurs a minimal process of secondary reactions and as a result of which are formed highly molecular sediments, pitches and coke in the reactor and heat exchange apparatus in the pyrolysis system and carbon oxides. A significant theoretical contributions is expected in the clarification of the interaction taking place in the copyrolysis between different hydrocarbons, in the determination of how, in the interaction, the overall kinetics of pyrolysis and the composition of products change.

We found promoting influence of tin on  $\text{LiO}/\text{Al}_2\text{O}_3$  catalyst as the oxidative coupling of the low molecular alkanes (methane) and of dimethylether to the higher hydrocarbons and ethers. We observed the mutual influence of hydrocarbons during copyrolysis of individual hydrocarbons reflecting in the rate of decomposition of individual components and in products distribution. It was similar during study of coke formation. The contribution is the decrease of coke formation during copyrolysis of studied hydrocarbons.

From soil and wastewaters contaminated by crude oil was isolated microbial consortium (*Pseudomonas putida*, *Klebsiella planticola*, *Xanthomonas maltophilia*) able to degrade naphthalene (0.3 g/L) and mixed culture (*Alcaligenes xylooxidans* and *Klebsiella pneumoniae*) degrading phenol substances (catechol, hydroquinone, resorcinol) at concentration 0.5 g/L. The optimal composition of basis nutrient elements (N, P, S) for the growth of microorganisms on naphthalene as a sole source of carbon was determined.

## V. COOPERATION

### A. Cooperation in Slovakia

SLOVNAFT, j.s.co., Bratislava

SLOVNAFT-VURUP, Bratislava

NAFTA, Gbely, j.s.co.

PETROCHEMA Dubová, j.s.co.

SPP (Slovak Gas Industry), Bratislava

EKOIL, j.s.co, Bratislava

Institute of Chemistry, Faculty of Natural Sciences, Comenius University, Bratislava



Department of Nuclear Physics and Technology, Faculty of Electrical Engineering, Bratislava

## B. International cooperation

Spolana, j.s.co., Neratovice, Czech Republic

- utilization of alfa-olefins

Ecole Nationale Supérieure de Chimie, Montpellier, France

- Xe-NMR-characterization of dealuminated zeolites

Institute of Physico-Chemistry and Electrochemistry, Academy of Sciences, Prague, Czech Republic

- Evaluation of zeolites by infra-red spectroscopy

- Determination of adsorption properties of ZSM-5 zeolites

## C. Membership in Domestic Organizations and Societies

Slovak Society of Industrial Chemistry, Bratislava

(E. Hájeková, M. Bajus, P. Daučík, P. Hudec, B. Liptáková, A. Smiešková, Z. Židek)

Slovak Society of Chemical Engineering, Bratislava

(P. Hudec, A. Smiešková, Z. Židek)

Slovak Zeolite Association

(P. Hudec - chairman, A. Smiešková, L. Šabo, Z. Židek)

## G. Visitors from Abroad

Prof. L. Zanzotto

University of Calgary, Calgary, Canada, September 2000 (7 days)

## H. Visits of Staff Members and Ph.D. Students in Foreign Institution

E. Hájeková

University of Calgary, Calgary, Canada, June – August 2000 (90 days)

## VI. THESES AND DISSERTATIONS

### A. Graduate Theses (MS Degree) for state examinations after five years of study (supervisors are written in brackets)

Chvojková M.:

Contents supervision of zinc, calcium, sulphur and phosphorus in oils (P. Daučík)

Kortišová A.:

Reological properties of vaselines and greases (J. Ambro)

Pechová A.:

Pyrolysis of communal and industrial wastes in the flow reactor (E. Hájeková)

Ráczová R.:

Hydrotreating of oil distillates (A. Smiešková)

Semanová S.:

Pyrolysis of communal and industrial wastes in the batch reactor (E. Hájeková)

Slišková M.:

Oxidative dehydrogenation of ethers (M. Bajus)

Vaňová M.:

Chromatographic determination of the middle distillates composition (P. Daučík)

Vlachovičová Z.:

Solubility of polymers and study of the transformation of fatty acids methylesters (M. Bajus)

## VII. PUBLICATIONS

### A. Journals (\*registered in Current Contents)

- 1] Bajus M.: Reformované a alternatívne palivá- súčasnosť a budúcnosť. Reformulated and Alternative Fuels – the Presence and the Future (in Slovak). Ropa, uhlie, plyn a petrochémia 43(2), 20-24 (2001).
- [2] Hájeková E., Bajus M., Lederer J., Novák V.: Coking of Different Gas Oil Fractions During Pyrolysis, Petroleum and Coal 43 (2), 98-100 (2001)
- [3] Hudec P., Smiešková A., Židek Z., Šabo L., Liptáková B: Deep-bed dealumination of ZSM-5 zeolites. Changes in structure and catalytic activity: Studies in Surface Science and Catalysis 135, 29-P-26/1-8 (2001)
- [4] Žikánová A., Kocirik M., Derewinski M., Sarv P., Dubský J., Hudec P., Smiešková A.: Mobilization of Surface Species during Transformation of Ethylene over HZSM-5 Catalysts., Studies in Surface Science and Catalysis 135, 24-P-10/1-8 (2001)

### B. Conferences (\*international conferences)

- [1]\* Bajus M.: Hydrocarbon Technologies for the Future, Current Trends in Oil and Petrochemical Industry. In: CD ROM Proceedings of the 40<sup>th</sup> International Petroleum Conference, Bratislava, Slovak Republic, September 17.-19., 2001, P-5
- [2]\* Daučík P., Hudec P., Ambro J., Židek Z.: Testing of low-temperature properties of diesel fuels. In: CD ROM Proceedings of the 40<sup>th</sup> International Petroleum Conference, Bratislava, Slovak Republic, September 17.-19., 2001, L-D-7
- [3]\* Daučík P., Hudec P., Ambro J., Židek Z., Leško J., Jakubík T: Methods of determination of diesel fuels composition. In: Proceedings of the 40<sup>th</sup> International Petroleum Conference, Bratislava, Slovak Republic, September 17.-19., 2001, L-D-6
- [4]\* Daučík P., Hudec P., Ambro J., Židek Z., Leško J., Jakubík T: Nitrogen compounds isolation and their identification in middle distillates. In: Proceedings of the 40<sup>th</sup> International Petroleum Conference, Bratislava, Slovak Republic, September 17.-19., 2001, P-D-26
- [5]\* Hájeková E., Bajus M., Lederer J., Novák V.: Coking of Different Gas Oil Fractions During Pyrolysis. In: CD ROM Proceedings of the 40<sup>th</sup> International Petroleum Conference, Bratislava, Slovak Republic, September 17.-19., 2001, P-E-37
- [6]\* Hudec P., Smiešková A., Židek Z., Stefankovicsová G., Daučík P., Šabo L., Ambro J.: Influence of Nitrogen Compounds on Color Degradation of Motor Fuels. In: Proceedings of the 40<sup>th</sup> International Petroleum Conference, Bratislava, Slovak Republic, September 17. – 19., 2001, L-D-5
- [7]\* Hudec P., Smiešková A., Židek Z., Stefankovicsová G., Daučík P., Šabo L., Ambro J.: Study of catalytic improvement of

- colour instability of middle distillates. In: Proceedings of the XXXIII. Symposium on Catalysis, Prague, Czech Republic, Nov. 5.-6. 2001, p.18
- [8]\* Liptáková B., Hronec M.: Oxidation of Benzene over Mixed Calcium-Copper hydroxyapatite catalysts. In: Proceedings of the XXXIII. Symposium on Catalysis, Prague, Czech Republic, Nov. 5.-6. 2001, p. 49
- [9]\* Smiešková A., Hudec P., Ráczová R., Šabo Ľ., Židek Z.: Comparison of Conventional and Y Zeolites Containing Hydrorefining Catalyst in Denitrogenation of Middle Fuel Distillates Derived from Different sources. In: Proceedings of the XXXIII. Symposium on Catalysis, Prague, Czech Republic, Nov. 5.-6. 2001, p. 54
- [10]\* Svitaň R., Ilkovič J., Biskupičová E., Bajus M.: Oxidative Coupling of Methane. Poster P-E-34. In: CD ROM Proceedings of the 40<sup>th</sup> International Petroleum Conference, Bratislava, Slovak Republic, September 17. – 19. , 2001
- [11]\* Svitaň R., Bajus M.: Membránové reaktory pre separáciu vodíka. Membrane reactors for hydrogen separation (in Slovak). In: CD ROM Proceedings of the 48<sup>th</sup> Conference of Chemical and Process Engineering, CHISA 2001, Srní, Šumava, Czech Republic, October 15.-18., 2001, V3.16.
- [12]\* Šabo Ľ., Hudec P., Smiešková A., Balážová K., Židek Z.: Mesoporous Materials as Support for Nickel Hydrogenation Catalyst. In: CD ROM Proceedings of the 40<sup>th</sup> International Petroleum Conference, Bratislava, Slovak Republic, September 17.-19., 2001, L-A-6
- [13]\* Šabo Ľ., Hudec P., Smiešková A., Balážová K., Židek Z.: Hydrogenation activity of Nickel Supported Mesoporous Materials., 1st. EFCAT School 2001, Prague, Czech Republic, March 27. - April 1. 2001, p.1
- [14]\* Šimon P., Okuliar J., Daučík P.: Practical Importance of the Kinetics of Induction Period. 28 International Conference of Slovak Society of Chemical Engineering. Tatranské Matliare, Slovak Republic, May 21. – 25. , 2001, L-44

#### D. Patents

- [1] Bajus M., Snopek P., Magač A., Kulka A., Kaščák S.: Spôsob aktivácie organických látok. Organic compounds activation (in Slovak), Sk 281993, (8.10.2001) Slovak Republic

#### E. Others

- [1] Bajus M.: Cesta zarúbaná paragrafmi. The route logged with paragraphs. (in Slovak) STOP Vol.31 č.25-26, (8-9) (2001)
- [2] Bajus M. a kolektív: Ekologické palivá, diskusia, názorové fórum o bionafté, Ecological fuels, discussion forum about biodiesel. (in Slovak) TREND, 11, 31, p. 8A - 9A.(2001).
- [3] Bajus M.: Telecast „Ekonomika Slovenska“. „Slovak economics“ (in Slovak), Vystúpenie v ST, Propagácia výsledkov výskumu o ekologických palivách č.3/2001 STV2 12.3.2001, repr. STV1, 17.3.2001.
- [4] Bajus M.: telecast "Mýtus o bionafté". „The mythos about biodiesel“. (in Slovak), Vystúpenie v ST, STV1, 6.7.2001

## DEPARTMENT OF PHYSICAL CHEMISTRY

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### I. STAFF

**Full Professors:**

Stanislav Biskupič, PhD, DSc; Peter Pelikán, PhD, DSc; Andrej Staško PhD, DSc

**Associate Professors:**

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**Assistant Professors:**

Vladimír Adamčík, PhD; Martina Bittererová, PhD; Róbert Klement, PhD; Ján Micanko, PhD; Jozef Polakovič, PhD; Štefan Pollák, PhD; Peter Rapta, PhD; Ján Reguli, PhD; Ľubomír Zalibera, PhD

**Research Fellows:**

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**PhD Students:**

Dana Dvoranová, Marek Fronc, Martin Polovka

**Technical Staff:**

Alojz Budoš, Imrich Csonka, Katarína Labudová, Marta Lintnerová, Miroslav Minarových, Štefan Miksai, Milan Štefunko, Mária Šuleková, Štefan Šurman

**Emeritus Fellows:**

Ján Mikuláš Lisý, PhD; Alexander Tkáč, PhD, DSc, Ladislav Valko PhD, DSc, Augustín Jurkovič

### II. TEACHING AND RESEARCH LABORATORIES

#### A. Teaching Laboratories

Laboratory for the Basic Course of Physical Chemistry  
Laboratory for the Advanced Course of Physical Chemistry  
Laboratory of Electronics  
Laboratory of UV-VIS and IR Spectroscopy

#### B. Research Laboratories

Laboratory of Differential Scanning Calorimetry  
Laboratory of EPR Spectroscopy  
Laboratory of Material Study and Light Scattering  
Laboratory of Molecular Distillation

#### C. Special Measuring Instruments

Electron Paramagnetic Resonance Spectrometer BRUKER ER 200D-SRC  
Differential Scanning Calorimeter DSC-7 Perkin-Elmer with an accessory for dynamic DSC

### III. TEACHING

#### A. Undergraduate study

1. Introductory courses

**3rd semester (winter)**

|  |         |                        |
|--|---------|------------------------|
| Physical Chemistry I.                        | (3-2 h) | S. Biskupič, A. Gatiaľ |
| Laboratory Practice in Physical Chemistry I. | (0-3 h) | J. Reguli              |

**4th semester (summer)**

|   |         |  |
|---|---------|--|
| Physical Chemistry II.                        | (3-2 h) | S. Biskupič, P. Kovařík, A. Gatiaľ, J. Antalík |
| Laboratory Practice in Physical Chemistry II. | (0-3 h) | P. Šimon                                       |

2. Advanced courses

**5th semester (winter)**

|  |         |                       |
|--|---------|-----------------------|
| Physical Fundamentals of Spectroscopic Methods | (2-2 h) | A. Staško, V. Brezová |
|--|---------|-----------------------|

**6th semester (summer)**

|                       |         |          |
|-----------------------|---------|----------|
| Biophysical Chemistry | (2-2 h) | M. Valko |
|-----------------------|---------|----------|

**7th semester (winter)**

|                     |         |            |
|---------------------|---------|------------|
| Chemical Physics I. | (2-1 h) | P. Pelikán |
|---------------------|---------|------------|

|   |          |                        |
|---|----------|------------------------|
| Thermodynamics  | (2-1 h)  | P. Šimon               |
| Kinetics and Catalysis                                    | (2-1 h)  | P. Kovařík             |
| Colloid Chemistry   | (2-0 h)  | J. Antalík             |
| Statistical Treatment and Evaluation of Experimental Data | (2-0 h)  | M. Breza               |
| Group Theory and Symmetry                                 | (2-0 h)  | M. Breza, V. Kvasnička |
| Special Laboratory Practice I                             | (0-8 h)  | P. Rapta               |
| <b>8th semester (summer)</b>                              |          |                        |
| Chemical Physics II.                                      | (2-1 h)  | S. Biskupič            |
| Solid State Physics                                       | (2-0 h)  | M. Breza               |
| Special Laboratory Practice II.                           | (0-6 h)  | P. Rapta               |
| Traineeship   |          |                        |
| Excursion   |          |                        |
| <b>9th semester (winter)</b>                              |          |                        |
| Molecular Spectroscopy                                    | (2-1 h)  | A. Staško              |
| Chemical Physics III.                                     | (2-0 h)  | A. Gatjal              |
| Special Laboratory Practice III.                          | (0-10 h) | P. Rapta               |

## IV. CURRENT RESEARCH PROJECTS

### A. Structure and Reactivity in Chemical and Biological Systems (Andrej Staško)

The research activity of our group is focused on the intermediates formed in various organic and aqueous systems, which are formed during photochemical and electrochemical processes and simultaneously monitored by different spectroscopic methods (EPR, UV/Vis, and NIR). One of the most investigated systems remains new carbon structures (fullerenes, nanotubes), where the formation of the corresponding anions is followed in the cathodic or photochemical reduction. Recently we expanded such studies also to the dimeric forms of  $C_{60}$  ( $C_{120}$ ,  $C_{120}O$ ). The results obtained bring new aspects in the follow up reactions of fullerene anions in the solutions.

To obtain a new quality of information we are developing in situ spectroelectrochemical techniques under a simultaneous exploitation of EPR, UV/Vis, NIR spectroscopy and cyclic voltammetry. These studies were recently expanded to the measurements at different temperatures, what enables an unambiguous assignment of the spectral data to the species generated in the electron transfer reactions and their follow up reactions with neighbourhood. This is frequently not possible if the experiments as electrochemical, optical or EPR measurements are carried out separately, especially if more unstable intermediates or complex spectroscopic data are expected. The technique developed was successfully applied in the fullerene investigations, reversible dimerisation of ion radicals and in the redox processes of new oligomeric and polymeric structures as candidates in sensor applications and as light emitting diode components.

The quantitative EPR spectroscopy remains a permanent problem due to the very limited reproducibility, as various parameters (position of the sample in the cavity, its shape, changing parameters of spectrometer and others) are very sensitively reflected in the integral intensity of EPR signals. To map and to eliminate these error sources an intensive research is carried out in numerous laboratories. Systematic investigations and a valuable contribution to this field was lately published from our laboratory, where the influence of the probe position, its size and other parameters were described enabling the elimination of many errors frequently neglected so far. The results obtained allow predict the change of EPR amplitude on the position and the shape of the sample.

The role of the radical processes is increasingly recognised not only in the living organisms but also in the foods, where the radical mechanisms are frequently responsible for their loosing quality. Based on this assumption, various methods to test the quality of foods were elaborated. We also started research in this field applying EPR spin trapping in the investigations of stability of beer probes from the Slovak and Czech market and then also from the German market and suggested a procedure enabling to compare and to predict the beer stability of various probes. Similarly we suggested and tested by now some procedures to evaluate the antioxidant - scavenging activity of wine probes.

### B. Development and Application of Computational Methods to the Study of Structure, Dynamics and Properties of Molecular Systems (Stanislav Biskupič)

1. A new method for generation of the relativistic Gaussian basis sets has been elaborated and implemented. The optimization method is based on the stochastic two-step procedure.

2. Theoretical treatment for calculation of the interaction energy of two closed shell systems and the molecular complex containing one open and one closed shell system has been formulated and applied in order to test the reliability of the proposed theory. New method is based on the 3rd order many body perturbation theory. The superposition error elimination was the subject of our investigations, too.

3. Precise calculations based on the MR SDCI method has been applied in order to obtain a good estimation of the potential hypersurface for HFF open shell molecular system with the aim to use it as a basic input for the future molecular dynamics studies. Sufficiently large active space has been used in all calculations.

4. Quantum chemical study of the azomethane decomposition has been done. Several kinetic parameters of the reactions under study were calculated.

5. Infrared spectra of selected organic compounds have been registered. Their interpretation and conformational analysis is based on the ab initio method with inclusion of the correlation energy.

6. Based on the newly developed theoretical treatment the calculation of the adiabatic and/or nonadiabatic corrections to the energy and vibrational frequencies has been done.

7. Periodic solid state systems have been studied within the originally reformulated theoretical treatments on the basis of the INDO type semiempirical hamiltonian.

8. The mutual influence between perturbation of the electronic structure of molecules and perturbations of regular

geometric arrangement of atoms in molecules has been studied. In systems with degenerate electronic states, the perturbations are due to vibronic interactions, whereas in cis-trans phosphazenes the perturbations are a consequence of non-equivalence of interatomic interactions.

### C. MATERIALS – Physico-chemical Methods of their Study and their Preparation (Peter Šimon)

The method for the evaluation of kinetic parameters of induction periods has been elaborated. The method enables to estimate the length of nonisothermal induction periods in the processes such as rubber curing, polymer and oil oxidation, freezing of undercooled liquids etc. The method is expected to be applied in the quality management and risk assessment in technological processes.

Degradation and stabilisation of PVC is studied both experimentally and theoretically. The attention is paid to the non-hazardous stabilizer mixtures based on tocoferyl acetate.

The thermochemical behaviour of selected complex compounds of Ni, Cu and Co has been studied from the point of view of their application as adhesion promoters in rubber curing.

The influence of glass transition and nonisothermal treatment of amorphous metal metals  $Fe_{100-x}B_x$  ( $13 < x < 21$ ) on the relative permeability, core-losses and magnetic induction has been investigated.

The processes occurring in foods and food packaging are modelled with the aim of hazard assessment in critical control points.

A method for the parameter evaluation in implicit and nonlinear models without the necessity of using any linearisation is suggested.

### D. Separation in Molecular Evaporator (Ján Cvengroš)

The research project is focused on the theory of molecular distillation, the development of the short-path evaporators with wiped film and on the applications of molecular distillation. The main results in 2001 are as follows:

1. Further development of the mathematical model of the molecular distillation comprising all till now known factors which influence the process. The model allows to evaluate the influence both process and construct parameters on the output and separation, to render the information about the unmeasurable parameters, to simulate different situations in the evaporator and to optimise the process. Using the model, the effect of entrainment separator was studied, as well as the feed temperature influence on the evaporator efficiency, the influence of the evaporating film hydrodynamics and the possibilities of divided condenser. Good agreement was achieved by comparison between experimental and model results.

2. The shape of RTD-curves from the study of profiled wipers with passage channels indicates that there are three different regimes in the liquid flow on the evaporating cylinder according the liquid load, peripheral speed of wiper, its construction and its sense of movement. The strand regime with the liquid flow downward along the screw tread at prolonged residence time is considered favourable for molecular distillation to perform efficient evaporation under gentle conditions at a lowered temperature.

3. Some interesting applications of molecular evaporators were developed (regeneration of used mineral oils, purification of some medicaments, PCB contaminated oils treatment, preparation of neutral methyl esters of vegetable oils and others).

### E. Calculation of Electron Structure of Solid State Materials and Synthesis of New Type of Materials (Peter Pelikán)

The program package for calculation of electron structure of solid state systems with translation symmetry were elaborated. The program uses complete Hartree-Fock operator including electron-electron interaction and he is applicable on the various levels of the theory (semiempirical methods, ab initio treatment, DFT theory). Up to now performed results were obtained using quasi-relativistic INDO method.

The proposed method is based on the calculation of finite clusters with modulo-cyclic boundary conditions. These conditions allow the Fourier transformation of the atomic orbitals to the Bloch functions, which follow the periodicity of the infinite crystal. After this transformation the secular problem transforms into a quasi-diagonal matrix what significantly decreases the computational time. Consequently, clusters up to 100,000 atoms can be calculated.

Calculation of such big clusters automatically incorporates long-distance interactions that may have dominant influence on the electron properties of the studied solid state systems. At the same time modulo-periodic conditions eliminate the so-called boundary effects (that limit the traditional cluster approach) that represent unsaturated bonds on the cluster boundaries.

Calculation of electron density is performed for tens of thousands points of the first Brillouin zone and provides the density matrix in a close neighborhood of the bulk limit.

The method incorporates the algorithm for inclusion of correlation effects that have a strong influence on the topology of the band structure and on the energy gap between the valence and conductive bands.

Automatic optimization of the geometry allows the calculation of various possible geometric arrangements in the solid state that can strongly influence physical and chemical characteristics of the studied systems.

### F. The Role of Trace Metals and Light in Camptothecin – Serum Albumin Interactions (NMR and EPR Studies) (Marián Valko)

The anticancer drug camptothecin (CPT) is a plant alkaloid that has recently gained approval for clinical trials as a treatment of gastric, rectum, and bladder tumors. The drug exists in two forms, a lactone form which is biologically active and a carboxylate form which is not. It has been shown that in the presence of human serum albumin (HSA) the drug converts to the biologically inactive form and therefore the liposomal stabilization of the lactone form of the drug is of primary importance. In this connection the high resolution NMR study is planned to elucidate the stabilization of the lactone form of the drug and the nature of the binding mode with HSA. It is generally believed that camptothecin activity occurs through a free radical mechanism. We also believe, that the role of trace metals is in particular important. Our preliminary results show that upon irradiation (365 nm light) copper(II)-CPT complex generates free radicals which may cause DNA damage to cancer cells. The aim of the proposed project is to further investigate a radical mechanism of the action of the drug.

### G. Charge Density Studies of 3d-element Complexes from X-Ray Diffraction Data (Jozef Kožíšek)

By studying the charge density of selected coordination compounds following questions could be elucidate:

1. Compounds which produce excellent quality crystals (potential low R-value could be reached) like

Bis[bis(methoxycarbimido)-aminato]Cu(II) complex is a good model for 3d-electron distribution at a special coordination number and homogeneous/heterogeneous coordination sphere.

2. In blue protein model compounds like [Cu(bite)(BF<sub>4</sub>)] and [Cu(bite)(BF<sub>4</sub>)<sub>2</sub>] the mechanisms and reason for special redox properties in biological systems are studied (so-called „blue proteins“).

3. In spin crossover system d-stacking of benzimidazole rings probably forms information channels responsible for interesting magnetic properties of these Fe(II) coordination compounds.

4. Asymmetric synthesis is fashionable and coordination compound like Ni-complexes of the Schiff base are catalysts. What is the reason for such high selectivity?

5. In unusual coordination polyhedron for Cu(II) the distribution of 3d-electrons should help to understand bonding properties.

#### H. Non-formal Education in Chemistry (Ján Reguli)

The aim of this project is to prepare supporting educational materials to help chemistry teachers in basic and secondary schools. In 2001 a coloured periodic table „Origin of the Names of Chemical Elements“ with accompanying booklet (28 pp.) was published. This material was approved by the Ministry of Education. Several other educational materials for secondary school teachers and for gifted students interested in chemistry were published (including the tasks for Chemistry Olympiad). Results of this project are summarised in the monograph „Non-formal Education in the Field of Chemistry“ (Vyd. STU 2001, 109 pp., in Slovak).

## V. COOPERATION

### A. Cooperation in Slovakia

Department of Histology, Faculty of Medicine, Comenius University, Bratislava

Department of Chemistry, Faculty of Pedagogy, University of Trnava, Trnava

Faculty of Natural Sciences, Comenius University, Bratislava

Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava

Faculty of Natural Sciences, University P. J. Šafárik, Košice

Department of Chemistry, Faculty of Industrial Technologies Púchov, University of Trenčín

Institute of Experimental Pharmacology, Slovak Academy of Sciences, Bratislava

Research Institute of Drugs Modra

EKOIL Bratislava

EKOTIPS Bratislava

DETOX Banská Bystrica

Duslo Šaľa

Q-CHEM Modra

OTEZA Martin

DAMT-MDT Martin

Slovak Hydrometeorological Institute, Bratislava

LikoSpol Bratislava

Research Institute of Chemical Fibres, Svit

### B. International Cooperation

Institut für Theoretische Chemie und Strahlenchemie, Universität Wien, Austria

- Ab initio calculations of potential energy surfaces of small molecules using multiconfiguration methods

Institut für Analytische Chemie, TU Dresden, Germany, Department of Chemistry, University of Oslo, Norway: Measurement

- Interpretation and theoretical calculation of vibrational IR and Raman spectra of some organic molecules.

University of Technology Darmstadt, SRN

- Crystal structures of organic and coordination compounds

Royal Institute of Technology, Stockholm, Sweden

- Molecular dynamics of N<sub>4</sub>

Max-Planck-Institut für Strömungsforschung, Göttingen, Germany

- Photodissociation of HNCO

State University of New York, Buffalo, USA

- FT calculations of blue proteins model compounds

School of Pharmacy and Chemistry, John Moores University, Liverpool, United Kingdom (Dr Harry Morris)

- Spectroscopy of transition metal compounds

Multifrequency EPR Center, Chemistry Department (Dr. Eric McInness)

University of Manchester, Manchester, UK

Chemistry Program, Roosevelt University, Chicago, USA (Assoc. Prof. Joshua Telsler)

NMR Center, Bremen University, Bremen, FRG (Prof. Dieter Leibfritz, NMR spectroscopy)

University of Poznan, Poland

IFW Dresden e. V., Dresden, Germany

- Novel EPR techniques, intermediates in electrochemical reactions

Institut für Makromol. Chemie, TU München, Germany

- Material for light diodes

Institute of Physical and Theoretical Chemistry, Technical University, Graz, Austria

- EPR spectroscopy, education

CIBA Spzialitetenchemie GmbH, Grenzach, Germany (Dr. Krajnik)

- Purification of products on molecular evaporator

Department of Instrumental and Analytical Science, UMIIST, Manchester, UK (Dr. Kvasnik)

- Development of fiberoptic distributed sensors for ammonia

University of Technology, Sydney, Australia (Dr.A.Ray, Dr.P.Thomas)

- Processes with induction period

VSCHT, Institute of Polymers, Czech Republic (Dr.Z.Vymazal)

- Nonisothermal degradation of PVC

Faculty of Chemistry, Technical University, Brno, Czech Republic

LUKAS Research, Prague, Czech Republic (Dr.R.Lukáš, Dr.L.Kalvoda)

- Development of fiberoptic distributed sensors for ammonia

Faculty of Chemical Technology, University of Pardubice, Czech Republic (Prof.Drdák)

- Modelling of microbial growth

University of Saskatchewan, Canada (Dr.R.Šilerová)

- Properties of thiol thin layers on gold particles

### C. Membership in Domestic Organisations and Societies

Slovak Chemical Society

Institute of Inorganic Chemistry, Slovak Academy

of Sciences - member of Scientific Board

(P. Pelikán)

Chemical Papers - member of Editorial board

(P. Pelikán)

Slovak Academic Society, Bratislava

(P. Pelikán)

Slovak Society of Chemical Engineers

(J. Cvengroš)

Slovak Vacuum Society

(J. Cvengroš)

Slovak Group for Thermal Analysis and Calorimetry

(P. Šimon)

### D. Membership in International Organisations and Societies

International Society for Theoretical

Chemical Physics, Germany

(S. Biskupič)

International ESR Society, USA

(S. Biskupič)

American Chemical Society, USA

(A. Staško)

American Oil Chemist's Society, USA

(J. Cvengroš)

Journal of Thermal Analysis and

Calorimetry – regional editor

(P. Šimon)

International Confederation

for Thermal Analysis and Calorimetry

(P. Šimon)

### F. International Scientific Programmes

1. NATO program for thermo-electric materials (P.Pelikán)

2. CEEPUS program – (Project SK-102) co-operation with University Graz (Austria), University Poznan (Poland), University Veszprém (Hungary), University Sofia (Bulgaria), Masaryk University Brno (Czech Republic), University Maribor (Slovenia), Bulgarian Academy of Sciences (Bulgaria), Pedagogical University Zielona Gora (Poland), Babes-Bolyai University Cluj (Romania). (A. Staško)

3. Charge Density Analysis of Transition Metal Complexes by Accurate X-Ray Diffractions Methods, NSF-CHE96155, SUNY Buffalo, USA, 1999-2002 (J. Kožíšek).

4. 1 year NATO Collaborative linkage grant LST.CLG.977743: „Protein binding and photochemistry of the anticancer drug camptothecin,“ (Marián Valko In collaboration with Dr. H. Morris, Liverpool and Prof. J. Telser, Chicago).

### G. Visitors from abroad

Prof. P. Janderka

Masaryk University Brno, Czech Republic, 14 days

Dr. K. Ranguelova

Bulgarian Academy of Sciences, Bulgaria, 14 days

The co-ordinators CEEPUS meeting (Project SK-102)

Prof. G. Grampp, University Graz (Austria), Prof. S. Lamperski, University Poznan (Poland), Prof. N. Yordanov, University Sofia (Bulgaria), Prof. J. Vřešťál, Masaryk University Brno (Czech Republic), Prof. A. Wieckowski, Pedagogical University Zielona Gora (Poland), Prof. I. Baldea, Babes-Bolyai University Cluj (Romania), 3 days.

Prof. P. Coppens

State University of New York, Buffalo, USA, 4 days.

Dr. Paul Thomas

University of Technology, Sydney, Australia, 1 month.

Dr. Frank Kvasnik

DIAS UMIST, Manchester, UK, 3 days

Dr. H. Morris

John Moores University, Liverpool, UK, 10.7.2001-4.8.2001

Prof. J. Telser

Roosevelt University, Chicago, USA, 19.7.-23.7.2001

Dr. Jesús García Díaz

28 days

Dr. Miriam Martinello

National University of Rio Cuarto, Argentina, 4 days.

### H. Visits of Staff Members and Postgraduate Students to Foreign Institutions

M. Bittererová

Royal Institute of Technology, Stockholm, Sweden, (12 months)

M. Breza

State University of New York, Buffalo, USA, September 2001 (23 days)

V. Brezová

Institute of Theoretical and Physical Chemistry, University Veszprém (Hungary) (10 days)

J. Kožíšek,

TU-Darmstadt, Germany, July-August 2000 (40 days)

J. Kožíšek

ECM-20 Conference, Atlanta, USA., August 2001 (6 days).

J. Kožíšek

DESY-HASYLAB, Hamburg, Germany (2x 6 days).

D. Dvoranová

University Poznan (Poland) (1 month)

R. Klement

Institut Charles Sadron, UPR 22-CNRS, 6, rue Bousisingault, F-67083 Strasbourg Cedex, France (9 months)

|           |   |
|-----------|---|
| P. Rapta  | IFW Dresden, Germany (3 months)                                     |
| I. Vrábek | University of Vienna, Austria, January-September 2001 (9 months)    |
| P. Šimon  | DIAS UMIST, Manchester, UK (5 days)                                 |
| P. Šimon  | University of Saskatchewan, Canada (1 month)                        |
| M. Valko  | John Moores University, Liverpool, UK August-September 2001(4 week) |

## VI. THESES AND DISSERTATIONS

### A. Graduate Theses (MS degree) for state examinations after five years of study (supervisors are written in brackets)

|                         |   |
|-------------------------|---|
| Fronc M.:               | Study of solid state electronic structure using exact X-ray diffraction data. (J. Kožíšek)  |
| Chalupková - Pírová K.: | Salt-aqueous oscillator. (V. Adamčík)   |
| Lichnerová E.:          | Redox properties of stobadine pyroindol derivatives investigated using spectroelectrochemical EPR and UV/visible techniques. (P. Rapta) |
| Okuliar J.:             | Oxidation of mineral oils and drugs – study of the non-isothermic induction period. (P. Šimon)  |
| Polovka M.:             | Radical intermediates formed during beer ageing. (V. Brezová)   |
| Slovák K.:              | Investigation of tocopherols influence in the stabilization mixtures for PVC. (P. Kovařík)  |
| Švorec J.:              | Forbidden transitions and their interpretation in the EPR spectra of copper(II) complexes. (M. Valko)                                   |

### B. Dissertations (PhD)

|           |   |
|-----------|---|
| E. Klein: | Study of the thermal degradation of polyvinyl chloride. |
|-----------|---|

### C. Dissertations (DSC)

|           |   |
|-----------|---|
| P. Šimon: | Kinetics of thermal degradation and stabilization of selected polymers. |
|-----------|---|

### D. Habilitation Thesis

|           |  |
|-----------|--|
| M. Mazúr: | Development of EPR techniques applied to the study of transition metal systems.                                |
| P. Rapta: | Radical intermediates in electrochemical redox reactions studied by in situ spectroelectrochemical techniques. |

## VII. PUBLICATIONS

### A. Journals (\*registered in Current Contents)

- [ 1]\* Baňacký P., Pelikán P., Valko M., Buchta S., Hanic F., Cigaň A.: Electron Paramagnetic Resonance of High-Tc Superconducting Composites YBa<sub>2</sub>Cu<sub>3-x</sub>Sc<sub>x</sub>O<sub>6±</sub>. J. Phys. Chem. B 105, 1943-1946 (2001).
- [ 2]\* Bishop D.W., Thomas P.S., Ray A.S. & Šimon P.: Two-stage kinetic model for the a-b phase recrystallisation in nickel sulfide. Journal of Thermal Analysis and Calorimetry 64, 201-210, (2001).
- [ 3]\* Bittererová M., Brinck T., Ostmark H.: Theoretical Study of the Singlet Electronically Excited States of N<sub>4</sub>. Chem. Phys. Lett. 340, 597-603 (2001).
- [ 4]\* Bittererová M., Ostmark H., Brinck T.: Ab initio study of the ground state and the first excited state of the rectangular (D<sub>2h</sub>) N<sub>4</sub> molecule. Chem. Phys. Lett. 347, 220-228 (2001).
- [ 5]\* Breza M., Lukeš V., Vrábek I.: On the dependence of optical properties on conformational changes in oligothiophenes I. Electron absorption spectra. J. Mol. Struct. (THEOCHEM) 572, 151-160 (2001).
- [ 6]\* Breza M., Šimon P. & Landl M.: On the dependence of spectra of NIR polymethine dyes on the central chromophore ring. Chemical Papers 55, 86-90, (2001).
- [ 7]\* Cvangroš J., Pollák Š., Micov M., Lutišan J.: Film wiping in the molecular evaporator. Chem. Eng. J, 81, 9-14 (2001).
- [ 8]\* Fáber R., Staško A., Nuyken O.: New blue crosslinkable polymers for organic light emitting devices. J. Macromol. Sci. – Pure Appl. Chem. A38, 353-364 (2001).
- [ 9]\* Hvastijová M., Kohout J., Buchler J.W., Katzenmeier H.W. Kožíšek J. & Didierjean C.: Crystallographic and Spectroscopic Evidence of O-Bonding in 3d-Metal Dicyanomethanidonitrite Complexes. Z. fur Naturforschung., 56b, 100-104 (2001).
- [10]\* Hvastijová M., Kohout J., Díaz, J.G., Kožíšek J. & Buchler J.W.: X-ray structural and spectroscopic investigation of cyanamidonitrate nickel(II) complexes with pyrazole type ligands. Transit. Metal Chem., 26, 4/5, 430-434 (2001).
- [11]\* Kavan L., Rapta P., Dunsch L., Bronikowski M. J., Willis P., Smalley R. E.: Electrochemical tuning of electronic structure of single-walled carbon nanotubes: in situ Raman and Vis-NIR study. J. Phys. Chem. B 105, 10764-10771 (2001).
- [12]\* Klein E., Kovařík P., Valko L.: Kinetic Study of Irganox E Antioxidants on Thermal Degradation of Poly(vinylchloride). Chemical Papers 55, 67-70, (2001).
- [13]\* Kožíšek J. Šafář P. & Langer V.: 1-[2(Dicarboxymethyl)-3-oxocyclopent-4-en-1-yl]pyrrolidin-1-ium bromide hydrate. Acta Cryst., E57, o775-o777 (2001).
- [14]\* Lukeš V., Breza M., Pálszegi T., Laurinc V., Vrábek I.: On the relation between conformational changes and optical properties in oligothiophenes 2. Linear and non-linear optical properties. Macromol. Theor. Simul. 10, 592-599 (2001).
- [15]\* Lukeš V., Breza M., Végh D., Hrdlovic P., Krajcovic J., Laurinc V.: Non-linear optical properties of new bridged bis-thienyls I.



- Pyrazine-based bridges. Theory, synthesis and spectra. *Synth. Metals* 124, 279-286 (2001).
- [16]\* Lukeš V., Vrábek I., Laurinc V., Biskupic S.: Ab initio study of the HF-H van der Waals complex. *J. Phys. Chem. A* 105, 7686-7692 (2001).
- [17]\* Lukeš V., Vrábek I., Laurinc V., Biskupic S.: Ab initio study of the Li-H<sub>2</sub> van der Waals complex. *Chem. Phys.* 271, 1-8 (2001).
- [18]\* Malkov A. V., Baxendale I. R., Bella M., Langer V., Fawcett J., Russell D. R., Mansfield D. J., Valko M., Košovský P.: Synthesis of new chiral 2,2'-bipyridyl-type ligands, their coordination to molybdenum(0), copper(II), and palladium(II), and application is asymmetric allylic substitution, allylic oxidation, and cyclopropanation. *Organometallics* 20, 673-690 (2001).
- [19]\* Marchalín Š., Cvopová K., Pham-Huu D.P., Chudík M., Kožíšek J., Svoboda I. & Dadčh A.: Novel syntheses of densely functionalized indolizines, di- and tetrahydroindolizines from 2-formyl-1,4-dihydropyridine systems based on cascade process. *Tetrahedron Letters*, 42, 5663-5667 (2001).
- [20]\* Mazúr M., Valko M., Morris H.: Influence of the movement of "over full-length cavity" cylindrical samples along the x-axis of a double TE<sub>104</sub> and single TE<sub>102</sub> rectangular cavity on the EPR signal intensity. An unusual effect analysis. *Anal. Chim. Acta* 443, 127-141 (2001).
- [21]\* Mazúr M., Valko M., Morris H.: Influence of the movement of cylindrical samples with variable internal diameter and variable length along the x-axis of a double TE<sub>104</sub> and single TE<sub>102</sub> rectangular cavity on the EPR signal intensity: A sample shape study. *Appl. Magn. Reson.* 20, 317-344 (2001).
- [22]\* Mikloš D., Segla P., Palicová M., Kopicová M., Melník M., Valko M., Glowiak T., Korabik M., Mrozinski J.: Synthesis, spectral and magnetic properties, and crystal structures of copper(II)-2-methylthionicotinate adducts with chelating ligands. *Polyhedron* 20, 1867-1874 (2001).
- [23]\* Omelka L., Ondrášová S., Dunsch L., Petr A., Staško A.: Radical products in the chemical oxidation of amines. An ESR study of secondary cation radicals from aniline and derivatives of 1,2-phenyldiamine. *Monatsh. Chem.* 132, 597-606 (2001).
- [24]\* Pelikán P., Košuth M., Biskupič S., Noga J., Straka M., Zajac A., Baňacký P.: Electron structure of polysilanes. Are these polymers one-dimensional systems? *Internat. J. Quantum Chem.* 84, 157-168 (2001).
- [25]\* Polakovič J.: Importance of chemomechanical processes for the applications of biaxially oriented polypropylene films in power capacitors. I. Phenomenological model of interaction. *Chemical Papers* 55, 1-6, (2001).
- [26]\* Rapta P., Dunsch L.: Dimerisation of organic radical ions and redox reactions of dimers as studied by temperature-dependent in situ ESR/UV-vis-NIR spectroelectrochemistry. *J. Electroanal. Chem.* 507, 287-292 (2001).
- [27]\* Rapta P., Dunsch L.: Conducting polymers at electrode surfaces as studied by in situ ESR/UV-Vis-NIR spectroscopy. *Synthetic Metals* 119, 409-410 (2001).
- [28]\* Siebert R., Schinke R., Bittererová M.: Spectroscopy of ozone at the dissociation threshold: Quantum calculations of bound and resonance states on a new global potential energy surface. *Phys. Chem. Chem. Phys.* 3, 1795-1798 (2001).
- [29]\* Šima J., Brezová V.: Mechanism of photoinduced processes in solutions of iodo iron(III) complexes containing Schiff base ligands. *Monatsh. Chem.* 132, 1493-1500 (2001).
- [30]\* Šima J., Lauková D., Brezová V.: Photoredox reactions of iodo iron (III) complexes containing tetradentate ligands. *Collect. Czech. Chem.* 66, 109-118 (2001).
- [31]\* Šimon P. & Kolman L.: DSC study of oxidation induction periods. *Journal of Thermal Analysis and Calorimetry* 64, 813-820, (2001).
- [32]\* Štolcová M., Kaszonyi A., Hronec M., Liptaj T., Staško A., Leško J.: Reaction of N-tert-butyl-2-benzothiazolesulphenamide with acetic anhydride in the presence of acids: II. Spectral studies. *J. Mol. Catal. A: Chem.* 172, 175-186 (2001).
- [33]\* Tarábek J., Wolter M., Rapta P., Plieth W., Maumy M., Dunsch L.: Functionalized conducting polymers for chemical sensors (in situ ESR/UV-Vis-NIR voltammetric study). *Macromol. Symp.* 164, 219-225 (2001).
- [34]\* Valko L., Klein E., Kovařík P., Bleha T., Šimon P.: Kinetic Study of Thermal Dehydrochloration of Poly(vinylchloride) in the Presence of Oxygen Catalytic Activity *European Polymer Journal* 37, 1123-1132, (2001).
- [35]\* Valko M., Morris H., Mazúr M., Rapta P., Bilton R. F.: Oxygen free radical generating mechanisms in the colon: do the semiquinones of vitamin K play a role in the aetiology of colon cancer? *Biochim. Biophys. Acta/Gen. Subj.*, 1527, 161-166 (2001).
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- [38] Gudmundson O., Gjendemsjo L.K., Cvengroš J.: Polynenasýtené mastné kyseliny radu n-3 v dietetických doplnkoch z rybích olejov. n-3 polyunsaturated fatty acids in marine oil supplements (in Slovak). *Bull. Potr. Výsk.* 40, 33-42, (2001).
- [39] Reguli J.: Od neformálneho vzdelávania k podpore školského vzdelávania v chémii. From Non-formal Education to the Support of School Chemical Education (in Slovak). *Acta Fac. Paed. Univ. Tyrnaviensis, Ser. D*, 4, 103-108 (2000); ISBN 80-88774-87-X.
- [40] Reguli J.: Úlohy z fyzikálnej chémie. Republikové kolo 37. ročníka CHO v kategórii A. Tasks for the Chemistry Olympiad (in Slovak). *Chemické rozhľady* 2 (1), 13-14, (2001); ISBN 80-88893-58-5.
- [41] Reguli J.: Riešenie a hodnotenie úloh z fyzikálnej chémie. Republikové kolo 37. ročníka CHO v kategórii A. Solution of the Tasks for the Chemistry Olympiad (in Slovak) *Chemické rozhľady* 2 (1), 35-38 (2001); ISBN 80-88893-58-5.
- [42] Reguli J.: Vybrané kapitoly z fyzikálnej chémie I. Základné termodynamické pojmy a zákony. Chapters in Physical Chemistry I. Basic Concepts and Laws of Thermodynamics (in Slovak). *Chemické rozhľady* 2 (1), 107-117 (2001); ISBN 80-88893-58-5.
- [43] Reguli J.: Úlohy z fyzikálnej chémie pre študijnú časť školského kola 38. ročníka CHO v kategórii A. Tasks for the Chemistry Olympiad (in Slovak). *Chemické rozhľady* 2 (3), 7-9 (2001); ISSN 1335-8391.
- [44] Reguli J.: Vybrané kapitoly z fyzikálnej chémie II. Fázové rovnováhy v jednozložkovej sústave. Chapters in Physical Chemistry II. Phase Equilibrium in one-component Systems (in Slovak). *Chemické rozhľady* 2 (4) 41-49 (2001); ISSN 1335-8391.

## B. Conferences (\*international conferences)

- [1]\* Baloghová Z., Mazúr M., Valko M., Baran P., Dlháň L., Valigura D.: Structure and EPR spectra of 1:1 copper complex with 2,2'-bipyridine-N,N'dioxide ligand. *Book of Abstracts*, p. 45, 18th International Conference on Coordination and Bioinorganic Chemistry, Smolenice, Slovak Republic, June, 4-8, 2001.

- [2]\* Baloghová Z., Mazúr M., Valko M., Baran P., Dlháň L., Valigura D.: Structure and EPR spectra of 1:1 copper(II) complexes with 2,2'-bipyridine-N,N'-dioxide ligand. Challenges for Coordination Chemistry in the New Century, Volume 5. (Melník M., Sirota A., Eds.) Slovak Technical University Press, Bratislava, 2001, p. 59-64. ISSN 1335-308X, ISBN 80-227-1539-5.
- [3]\* Bishop D.W., Thomas P.S., Ray A.S. & Šimon P.: Crystallization of Nickel Sulfide by Non-isothermal Cooling. In: Challenges for Coordination Chemistry in the New Century, Ed. M.Melník & A.Sirota, STU press, Bratislava 2001, pp.397-402.
- [4]\* Bírová A., Švajdenka E., Cvengroš J., Dostálíková V.: Content of vegetable oil methyl esters in mixed fuels. Proc. 40th Int. Petroleum Conf., P-D27, 17.-19.9.2001, Bratislava, SR.
- [5]\* Bírová A., Švajdenka E., Cvengroš J., Dostálíková V.: Stanovenie hmotnostného podielu metylesterov v zmesných palivách. Determination of methyl ester fraction in mixed fuels. Zborník príspevkov, 53. zjazd chem. spoločností, B. Bystrica, 3.-6.9.2001, str. 266-267, ISBN 80-89029-23-X.
- [6]\* Biskupič S.: Fitovanie hyperplôch potenciálnej energie. Zborník príspevkov 53. zjazdu chemických spoločností, B. Bystrica, 3.-6. september 2001, p. 291-292.
- [7]\* Breza M., Kožíšek J., P. Coppens: DFT studies of blue protein copper compounds. Challenges for Coordination Chemistry in the New Century. Monograph series of the International Conference on Coordination Chemistry (Eds. M. Melnik, A. Sirota), Slovak Technical University Press, Bratislava 2001, Slovakia, pp. 115-120, ISBN 80-227-15.
- [8]\* Brezová V., Valko M., Breza M., Dvoranová D., Morris H.: The role of copper(II) in the anticancer action of irradiated camptothecin. 14th International Symposium on the Photochemistry and Photophysics of Coordination Compounds, Veszprém, Hungary, July 7 – 12, 2001, p. 57.
- [9]\* Brezová V., Valko M., Mazúr M., Morris H.: The role of trace metals in the photochemistry of anticancer drug camptothecin. Book of Abstracts, p. 40, 18th Conference on Coordination Chemistry, Smolenice, Slovak Republic, June, 4-8, 2001.
- [10]\* Brezová V., Valko M., Breza M., Mazúr M., Dvoranová D., Morris H., Telsler J.: The role of copper (II) in the anticancer action of irradiated camptothecin. Challenges for Coordination Chemistry in the New Century, Volume 5. (Melník M., Sirota A., Eds.) Slovak Technical University Press, Bratislava, 2001, p. 233-238. ISSN 1335-308X, ISBN 80-227-1539-5.
- [11]\* Cvengroš J., Cvengrošová Z., Hóka C.: Transesterification of vegetable oils to methyl esters and determination of conversion by TLC method. Proc. 40th Int. Petroleum Conf., P-D24, 17.-19.9.2001, Bratislava, SR.
- [12]\* Díaz J.G., Hvastijová M., Kožíšek J.: Cyanamidonitrate-copper(II), nickel(II) and cobalt(II) complexes of imidazole and pyrazole ligands. 20th ECM, Krakow 2001, p.344, Poland.
- [13]\* Dunsch L., Rapta P.: Dimerisation of electrochemically generated radical ions as studied by in situ ESR/UV-Vis-NIR spectroelectrochemistry at different temperatures. GDCh-Jahrestagung Chemie 2001, 23.-29. 9. 2001, Würzburg, Germany, Kurzreferate AEL ETR-004, p. 53.
- [14]\* Dunsch L., Staško A., Gromov A., Rapta P., Bartl A.: In situ spectroelectrochemistry of C60 and its Dimers: A Quantitative Study at Different Temperatures. Meeting Abstracts, The 199th Meeting of The Electrochemical Society, Washington, D. C., USA, March 25-30, 2001, Abstract No. 677.
- [15] Dvoranová D., Mazúr M., Brezová V., Staško A.: EPR study of metal doped TiO2 photocatalysts. Abstracts of RAMIS 2001, XIX International Seminar on Modern Magnetic Resonances, Poznan-Bedlewo, Poland, 6-10 May 2001, P-14.
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- [19]\* Hvastijová M., Kohout J., Kožíšek J. & Jäger L.: Cyanamidonitrate Complexes of Ni(II), Co(II) and Cu(II) with Pyrazole Ligands. Proc.18 CCC, 139-96, 2001, Smolenice-Bratislava.
- [20]\* Klein E., Kovářík P., Spišák R.: Štúdium teplotnej závislosti vplyvu tokoferoacetátu na termickú degradáciu PVC. 53. Zjazd Chemických spoločností, Banská Bystrica, 3.-6.9.2001, Zborník príspevkov.
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- [23]\* Lisý J.M., Biskupič S.: Kalibrácia metódou najmenších štvorcov. Calibration by the Least Squares Method (in Slovak). Zborník príspevkov 53. zjazdu chemických spoločností, B. Bystrica, 3.-6. september 2001, p. 289-290.
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- [27]\* Mazúr M., Valko M.: VO(II) EPR spectroscopy of sol-gel process. Book of Abstracts, p. 108, 18th Conference on Coordination Chemistry, Smolenice, Slovak Republic, June, 4-8, 2001.
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- [29]\* Mazúr M.: Quantity in magnetic resonance spectroscopy. Part 4. Book of Abstracts 16th NMR Valtice, Central European NMR Discussion Groups, Valtice, Czech Republic, 23. - 25. 4. 2001, p. 45.
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- [37]\* Polakovič J.: Aplikácia elektroanalytickej metódy na štúdium nadmolekulovej štruktúry vody. Moderní elektroanalytické Metódy XXI. SES Logis s.r.o. Ústí nad Labem ve spolupráci s Ústavem fyzikální chemie AV ČR Praha, 24.-26.4, 2001, Nedvedice u Nového Města na Morave.
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- [41]\* Reguli J., Linkešová M., Slanicay J: Pôvod názvov chemických prvkov. Origin of the Names of Chemical Elements(in Slovak). Zborník príspevkov 53. zjazdu chemických spoločností, Banská Bystrica, 3.-6. 9. 2001. 1. diel, str. 164-165 (2001).
- [42]\* Slovák K., Kovařík P., Klein E., Gatial A.: Štúdium vplyvu tokoferolu a tokoferoacetátu na tepelnú degradáciu PVC metódou Ramanovej spektroskopie. 53. Zjazd Chemických spoločností, Banská Bystrica, 3.-6.9.2001, Zborník príspevkov.
- [43]\* Staško A., Brezová V., Mazúr M., Malík F.: Free radicals scavenging activities of wines and characterization of beer stability (EPR spin trapping study). Book of Abstracts, p.56, 7th International workshop EMARDIS and APPLIED EPR, Sofia, Bulgaria, June, 09-18, 2001.
- [44]\* Šimko P., Šimon P., Belajová E.: Využitie vlastností plastových obalových materiálov na znižovanie koncentrácie benzo(a)pyrénu v rastlinných olejoch. V. medzinárodná konferencia, Obalové dny 2001, Zborník prednášok, Brno, 20.-21. 11. 2001, hotel Holiday Inn.
- [45]\* Šimon P., Okuliar J. & Daučik P.: Practical importance of the kinetics of Induction periods. 28th International Conference of Slovak Society of Chemical Engineering, Tatranské Matliare.

### C. Books and Textbooks

- [ 1] Reguli J. :Neformálne vzdelávanie v oblasti chémie. Non-formal Education in Chemistry (in Slovak). Vydavateľstvo STU, Bratislava 2001, 109 pp.; ISBN 80–227–1553–0.
- [ 2] Reguli J., Linkešová M., Slanicay J: Pôvod názvov chemických prvkov. Origin of the Names of Chemical Elements(in Slovak). FCHPT STU Bratislava 2001, 28 pp.

### E. Other Publications

- [ 1] Reguli J.: Fyzikálna chémia. Letná škola chemikov, kat. B. Physical Chemistry for the Summer School of Chemistry (in Slovak). IUVENTA, Bratislava, 2001, 20 str.
- [ 2] Reguli J.: Fyzikálna chémia. Letná škola chemikov, kat. C. Physical Chemistry for the Summer School of Chemistry (in Slovak). IUVENTA, Bratislava, 2001, 22 str.

## DEPARTMENT OF PHYSICAL EDUCATION

### Head of the Department

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### I. STAFF

#### Assistant Professors:

Peter Bartok, Július Fehér, Viliam Lendel, PhD, Jiřina Moravcová, Dalma Sochorová, Ivan Turčáni

#### Technical Staff:

Gabriela Boršányiová

### II. TEACHING AND RESEARCH LABORATORIES:

Gym 14x21 m – ground /volleybal, basketball, football/

Two Body Building rooms 15x5 m and 10x5 m

### III. TEACHING:

|                             |       |  |
|-----------------------------|-------|--|
| Aerobic                     | (2 h) | D. Sochorová                                     |
| Kalanethics                 | (2 h) | D. Sochorová                                     |
| Harmonic gymnastics         | (2 h) | D. Sochorová                                     |
| Healing gymnastic           | (2 h) | D. Sochorová                                     |
| Athletic sport              | (2 h) | V. Lendel  |
| Basketball                  | (2 h) | P. Bartok  |
| Football                    | (2 h) | P. Bartok  |
| Handball                    | (2 h) | M. Bobřík  |
| Body building               | (6 h) | M. Bobřík, P. Bartok, V. Lendel,<br>J. Moravcová |
| Swimming                    | (2 h) | J. Fehér, I. Turčáni                             |
| Canoeing and kayak          | (4 h) | M. Bobřík  |
| Volleyball                  | (2 h) | J. Moravcová                                     |
| Winter sports camp /skiing/ |       | M. Bobřík, J. Fehér                              |
| Summer sports camp /        |       | M. Bobřík, J. Fehér                              |

### IV. RESEARCH PROJECT:

State of Physical and Motor Development of Undergraduates of FCHFT STU in Bratislava (Viliam Lendel)

### V. COOPERATION IN SLOVAKIA:

Faculty Physical Education and Sport of the Comenius University, Bratislava;

Research Institute of Physical Culture, Bratislava;

Institute of History, Slovak Academy of Sciences, Bratislava.

### VI. PUBLICATIONS:

#### A. Journals

#### B. Conferences (\*international conferences)

- [1]\* Bobřík, M.: Nemci na Slovensku a slovenská otázka počas a po skončení prvej svetovej vojny (1916-1919), s. 105-112. Germans in the Slovakia and the slovaks Question during and after the I. World War (1916-1919) In: Mommsen, H., Kováč, D., Malíř, J., Marková, M.: První světová válka a vztahy mezi Čechy, Slováky a Němci. The First World War and the Conections between the Czechs, Slovaks and the Germans. Matices moravská Brno 2000. Česko-německá komise historiku, česká sekce 2000, ISBN 80-902304-8-2. Publikáciu financovalo Ministerstvo zahraničných vecí Českej republiky
- [2] Bobřík, M., Lendel, V.: Stav telesného a funkčného rozvoja poslucháčov CHTF STU v Bratislave. State of Physical and Functional Development of Undergraduates of CHTF STU in Bratislava In: Optimalizácia zaťaženia v telesnej a športovej výchove. Optimisation of the load in physical and sport education. Bratislava, 23.5.2001, s. 24-29. ISBN 80-227-1541-7.
- [3]\* Bobřík, M., Lendel, V.: Telesné a funkčné ukazovatele rozvoja poslucháčov FCHPT v Bratislave. Physical and Functional Parameters of Undergraduates of FCHPT STU in Bratislava. In: Telesná výchova, šport, výskum na univerzitách. Physical Education, Sport, Research on the universities. Zborník referátov z medzinárodnej konferencie, Bratislava 2001, s. 45-50. ISBN 80-227-1605-7.
- [4]\* Bobřík, M.: Problémy telesnej výchovy na VŠ v SR cez prizmu posledného desaťročia. Problems of physical education on the universities in the SR and view of last ten yers. In: Perspektívy školskej telesnej výchovy a športu pre všetkých v SR. Perspectivs of physical education and sport for all in the SROV. Zborník z celoslovenského vedeckého seminára, Bratislava

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- [5]\* Lendel, V.: Skúsenosti, problémy a perspektívy vyučovania telesnej výchovy na Fakulte chemickej a potravinárskej technológie STU v Bratislave. Experiences, problems and pespectieves of teaching physical education at Faculty chemical and foods technology STU in Bratislava. In: Perspektívy školskej telesnej výchovy a športu pre všetkých v SR. Zborník z celoslovenského vedeckého seminára, Bratislava 2001, s. 62-68. ISBN 80-89075-01-0.

## DEPARTMENT OF PLASTICS AND RUBBER

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### I. STAFF

**Full Professor:**

Dušan Bakoš, PhD, DSc

**Associate Professors:**

Ivan Hudec, PhD; Viera Chrástová, PhD; Gabriela Kyselá, PhD; Eugen Špirk, PhD

**Assistant Professor:**

Pavol Alexy, PhD

**Senior Research Fellow:**

Viera Khunová, PhD

**Research Fellow:**

Ľudmila Černáková, PhD

**PhD Students:**

Gabriela Crkoňová; Lenka Hajdučíková; Denisa Koniarová; Miroslav Kršiak; Henrich Krump; Lenka Precnerová; Petra Volfová

**Technical Staff:**

Mária Dočolomanská, Viera Godályová, Božena Lebočová, Mária Pekarovičová, Anna Tatarková

### II. TEACHING AND RESEARCH LABORATORIES

Laboratory of Polymer Synthesis

Laboratory of Polymer Solutions

Laboratory of Polymer Modification

Laboratory of Thermal Analysis

Laboratory of Polymer Rheology

Laboratory of Electron Microscopy

Laboratory of Polymer Processing and Estimation of its Mechanical and Physical Properties

Laboratory of Biomaterials

### III. TEACHING

#### A. Bacalarate Study

**5<sup>th</sup> semester (autumn)**

|  |         |                   |
|--|---------|-------------------|
| Macromolecular Chemistry                 | (2-0 h) | Chrástová         |
| Corrosion and Material Surface Treatment | (2-2 h) | Chovancová, Špirk |

**6<sup>th</sup> semester (spring)**

|                         |         |                           |
|-------------------------|---------|---------------------------|
| Technology of Materials | (2-0 h) | Hudec, Marcinčin, Majling |
| Technological Project   | (0-4 h) |                           |

#### B. Graduate Study

**7<sup>th</sup> semester**

|  |         |                              |
|--|---------|------------------------------|
| Polymer Physics                          | (2-2 h) | Cifra, Krištofič, Šutý       |
| Colloids and Interfaces                  | (2-1 h) | Bakoš, Mikula                |
| Laboratory from Macromolecular Chemistry | (0-8 h) | Černáková, Volfová, Crkoňová |
| Macromolecular Chemistry II              | (2-1 h) | Chrástová                    |
| Production and Processing of Plastics    | (3-0 h) | Hudec                        |
| Production and Processing of Rubber      | (3-2 h) | Kyselá                       |

**8<sup>th</sup> semester**

|  |         |   |
|--|---------|---|
| Additives for Plastics                           | (2-0 h) | Hudec   |
| Biotechnological Polymers                        | (2-0 h) | Bakoš   |
| Methods of Polymer Characterisation              | (2-0 h) | Černáková                                       |
| Design of Experiments                            | (1-1 h) | Alexy   |
| Laboratory from Production of Polymers           | (0-8 h) | Alexy, Kyselá, Krump, Kršiak                    |
| Production, Properties and Processing of Plastic | (2-0 h) | Hudec (for students of Faculty of Architecture) |

**9<sup>th</sup> semester**

|                               |         |         |
|-------------------------------|---------|---------|
| Polymer Processing            | (3-1 h) | Špirk   |
| Polymer Blends and Composites | (2-0 h) | Khunová |

|  |          |                             |
|--|----------|-----------------------------|
| Polymer Recycling and Waste Disposal   | (2-0 h)  | Špirk, Hudec, Khunová       |
| Polymer Testing                        | (0-2 h)  | Alexy                       |
| Laboratory from Processing of Polymers | (0-10h)  | Alexy, Hudec, Kršiak, Krump |
| <b>10<sup>th</sup> semester</b>        |          |                             |
| Diploma work                           | (0-27 h) |                             |

#### IV. CURRENT RESEARCH PROJECTS

##### A. Study of Synthesis of Crosslinked Polymers and their Properties (Viera Chrástová)

The project deals with synthesis of functionalized poly(styrene)/poly(butyl acrylate) dispersions with core-shell morphology of latex particles. The functional monomers especially N-methylol acrylamide and N-izobutoxy methylacrylamide are used at the course of two step emulsion polymerization for introduction of reactive groups into polymer chains. The influence of crosslinking reactions on colloidal characteristics of such modified dispersions and mechanical properties of their film are studied with the aim to obtain dispersion with application properties suitable for the formulation of ecological paints.

The crosslinking of unsaturated elastomers in the presence of amine-free accelerators is investigated, too. These accelerators do not form carcinogenic N-nitrosamines. The study is predominantly concerned with the research of the ageing-resistant behaviour of the natural rubber vulcanizates cured in the presence dialkyldithiophosphates or their combinations with thiazoles. The eventual ageing resistance was evaluated on the base of the changes of the primary properties of cured materials and on the changes of the arrangement of the network.

##### B. Polymer Mixtures, Composites and Recycling (Eugen Špirk)

The aim of the research project is the study of correlation between the structure, physical - mechanical, rheological and thermal properties of composites with a high content of soft and hard magnetic fillers based on thermoplastic and elastomeric matrix.

In the region of rubber blends the attention is oriented on following environmental problems:

- the formulation of rubber blends recipes from the viewpoint of nitrosoamine free cured system
- the applications of grinding rubber in polymer blends.

Further the research works are oriented on the reactive processing of particulate polymer composites based on the inorganic fillers and thermoplastic polymer matrix. The objective of this part is to identify effective modifier enable moulding of the composite with improved performance properties, as well as the effect of the reactive modifier on the interphase structure development.

The main research effort in the field of polymer recycling is aimed to the development of an environmentally viable and economically effective mode of improving mechanical and rheological properties of recycled thermoplastic waste.

##### C. The study of the macromolecular systems of hyaluronic acid with biologically active substances for biomaterial applications (Dušan Bakoš)

The scientific aims of the project are in developing the biosynthetic skin substitute, which is able to be definitely incorporated in body. The study results of the basic properties of biopolymers of extracellular matrix, collagen and hyaluronic acid. The developed membranes with excellent biological and mechanical properties are chemically modified to synchronise biodegradation and wound healing.

The preparation of the complex membrane based on collagen and hyaluronan was standardised on the basis of cytotoxicity and biodegradability testing and other properties. The pharmacological documentation was elaborated for clinical trial as skin covering, as well.

Based on received approval for the clinical trial, new application possibilities of the membrane were studied. Perspective applications rise in guide tissue regeneration in stomatology, as an antiadhesive membrane in orthopaedic surgery and skin covering with a possibility of controlled release of bioactive substances.

##### D. The development of ecologically acceptable flame retardant magnesium hydroxide based polymer composites (Viera Khunová)

The project aims to develop application specific halogen free flame retardant composites based on magnesium hydroxide and thermoplastics materials. This is being achieved via reactive processing that results in modification of the interfacial region between the filler particle surface and the polymer matrix.

The main research and experimental effort of the project is focused on optimisation of reactive processing conditions of modified polyolefine/magnesium hydroxide composites and their evaluation in relation to end-use properties. It was found, that under the determined optimum conditions, mechanical properties increased not only beyond that of the unmodified composite but also beyond the equivalent yield values of the unfilled matrix. The enhancement of major mechanical properties, i.e., tensile strength, elongation to break and impact strength, exceed the improvement afforded by current organic coupling agent pre-treatment systems.

The project is supported by British Council in Bratislava, the collaborative partner is the Manchester Metropolitan University, Manchester, UK.

##### E. New generation of inks for rotogravure printing (Viera Khunová)

The project is focused on formulation of polymer based hot melt inks (HMI) for rotogravure printing with specific demand on their physical stage. The significance of developed hot melt ink when compared to current toluene based ink is that they neither produce liquid nor volatile waste to pollute the environment.

On going phase of the project research is focused on rheological behavior, characterisation of polymer/pigment interphase, as well as kinetics of melting and solidification process.

The project is supported by NATO science program, the collaborative partner is the Western Michigan University, MI, USA.

## V. COOPERATION

### A. Cooperation in Slovakia:

Chemolak, a.s. Smolenice  
 Rubber Research Institute, Matador, a.s. Púchov  
 Research Institute of Processing and Application of Plastics, a.s. Nitra  
 Polymer Institute, Slovak Academy of Sciences, Bratislava  
 Research Institute of Chemical Technology, a.s. Bratislava  
 Matador, a.s. Púchov  
 Vegum, a.s. Dolné Vestenice  
 Plastika, a.s. Nitra  
 Slovnaft, a.s., Bratislava  
 NCHZ, a.s., Nováky  
 SELEKT a.s. Bučany  
 Orthopedical Clinic, School of Medicine, Comenius University, Bratislava  
 Burn Department and Skin Bank, Ružinov Hospital, Bratislava  
 Institute of Medical Biology, Faculty of Medicine, UK, Bratislava

### B. International Cooperation:

Martin Luther University of Halle - Wittenberg, Institute of Materials Science, Merseburg, Germany  
 - Modification of Polymers and Polymer Processing  
 Technical University of Szczecin, Institute of Material Engineering, Szczecin, Poland  
 - Chemical and Physical Modification of Polymers  
 Poznań University of Technology, Institute of Materials Technology, Poznań, Poland  
 - Testing and Processing of Rubber Blends and Reinforcing Materials  
 Western Michigan University, Kalamazoo, USA  
 - The development of new generation of hot-melt inks for rotogravure printing  
 The Manchester Metropolitan University, Faculty of Science and Engineering, Manchester, U. K.  
 - Reactive Processing of Particulate Polymer Composites  
 University of Minho, Department of Polymer Engineering, Guimarães, Portugal  
 - Development of biomaterials  
 University of Pisa, Department of chemistry and Industrial Chemistry, Pisa, Italy  
 - Biodegradable Plastics  
 Clinica Puerta de Hierro, Cirugia Experimental, Madrid, Spain  
 - Chemical Modification and Biocompatibility  
 - Testing of Collagen Membranes  
 National University of Singapore  
 - Testing of hybrid polymer membranes  
 Polymer Institute Brno, Czech Republic  
 - Testing of Polymers

### C. Membership in International Organisations and Societies:

European Biomaterial Society, Italy (D. Bakoš)

### G. Visitors from Abroad:

|                             |  |
|-----------------------------|--|
| Dr. Ivan Kelnar             | Institute of Macromolecular Chemistry, Prague, (2 days)  |
| Prof. Eduardo Jorge-Herrero | Clinica Puerta de Hierro, Cirugia Experimental, Madrid, Spain (5 days)                                       |
| Dr. Evelyn Dayss            | Martin Luther University of Halle - Wittenberg, Institute of Materials Science, Merseburg, Germany (5 days)  |
| Dipl. Ing. Sybill Illisch   | Martin Luther University of Halle - Wittenberg, Institute of Materials Science, Merseburg, Germany, (5 days) |
| Dr. Jaroslav Kučera         | Polymer Institute Brno, Czech Republic, (1 day)  |
| Dr. Eva Nezbedová           |  |
| Dr. Josef Křivánek          |  |

### H. Visits of Staff Members and Postgraduate Students to Foreign Institutions:

|                              |   |
|------------------------------|---|
| P. Alexy, I. Hudec, E. Špírk | Martin Luther University of Halle-Wittenberg, Institute of Materials Science, Merseburg, Germany, June 2001, (5 days)   |
| D. Bakoš                     | BPPT, Agency for the Assessment and Application of Technology, Jakarta, Indonesia (7 days)<br>Summer School of Biomaterials, Alvor, Portugal (14 days)<br>University of Bahrain and Gulf University, Manama, Bahrain (8 days) |
| I. Hudec                     | ICS-UNIDO, Trieste, Italy (4 days)<br>Polymer Institute Brno, Czech Republic, November 2001, (1 day)<br>Politechnika Szczecińska Szczecin, Poland, November 2001, (3 days)  |
| I. Hudec, P. Alexy           | 15 <sup>th</sup> International Trade Fair for Plastics and Rubber, Dusseldorf, Germany, October 2001, (4 days)  |
| V. Khunová                   | The Manchester Metropolitan University, Faculty of Science and Engineering, Manchester, U. K., January 2001, (10 days)  |



Western Michigan University, Department of Paper and Printing  
Kalamazoo, MI, USA, January-February 2001 (4 weeks)  
Politechnika Szczecińska Szczecin, Poland, November 2001, (4 days)  
Universität Gesamthochschule, Kassel, Germany, November 2001, (3 days)

## VI. THESES AND DISSERTATIONS

### A. Graduate Theses (MS Degree) for state examinations after five years of study (supervisors are written in brackets):

|                 |   |
|-----------------|---|
| Cíbk B.:        | Evaluation of filler activity in rubber mixtures (E. Špírk)   |
| Figura A.:      | Influence of crosslinking in solution on the polyolefine properties (I. Chodák)                                     |
| Figura T.:      | The modification of dynamic-mechanical properties of rubber mixtures (E. Špírk)                                     |
| Kozlík R.:      | Utilisation of collagen hydrolysate in polymer blends (I. Hudec)  |
| Martisovic J.:  | Study of properties of functionalized poly(styrene)/poly(butyl acrylate) dispersions (L. Černáková)                 |
| Rehák L.:       | Utilisation of reactive modifiers for preparation of micro and nanoscale polymer composites in melt (V. Khunová)    |
| Práznovská B.:  | Surface plasmochemical treatment of reinforcing materials for tire construction (I. Hudec)                          |
| Vanovčanová Z.: | Study of structure and properties of PVAL modified with collagen hydrolysate (D. Bakoš)                             |
| Perinová Z.:    | Synthesis and properties of poly(styrene)/poly (butyl acrylate) dispersions applicable for coatings. (V. Chrástová) |
| Precnerová L.:  | Development of PVAL–collagen hydrolysate blends for film blowing production (P. Alexy)                              |
| Sulyoková A.:   | The influence of phosphoric accelerators on the sulphur vulcanisation of natural rubber (G. Kyselá)                 |

### B. Dissertations (PhD)

|                 |   |
|-----------------|---|
| Crkoňová G.:    | The study of environmentally degradable blends of plastics with biopolymers (D. Bakoš)                                    |
| Hajdučiková L.: | The study of transport processes of biologically active compounds in complex biopolymer membrane (D. Bakoš)               |
| Koniarová D.:   | The study of macromolecular compositions based on biopolymers for biomaterials application - external form (D. Bakoš)     |
| Kršíak M.:      | Utilisation of collagen hydrolysate in polymer blends (D. Bakoš)  |
| Krump H.:       | Surface treatment of textile reinforcing materials for tire construction (I. Hudec)                                       |
| Reksová V.:     | Surface plasmochemical treatment of reinforcing materials for tire construction (I. Hudec)                                |
| Volfová P.:     | The effect of synthesis and formulation additives on the properties of polymer-styrene-acrylate dispersion (V. Chrástová) |

## VII. PUBLICATIONS

### A. Journals (\*registered in Current Contents)

- [1]\* Alexy P., Bakoš D., Crkoňová G., Kolomazník K., Kršíak M.: Blends of polyvinylalcohol with collagen hydrolysate: thermal degradation and processing properties, *Macromol. Symp.*, Vol. 170, 41-49, (2001)
- [2] Alexy P., Košíková B., Crkoňová G., Kozánková J., Martiš P., Precnerová L.: Effect of EVA copolymers on morphology and mechanical properties of polyethylene-lignin blends, *Ropa, uhlíe a petrochémia*, 43(1), 42-45, (2001)
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**B. Conferences (\*international conferences)**

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**C. Patents**

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## DEPARTMENT OF INFORMATION ENGINEERING AND PROCESS CONTROL

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### I. STAFF

**Full Professor:**

Ján Mikleš, PhD, DSc;

**Associate Professors:**

Monika Bakošová, PhD; Ján Danko, PhD; Ján Dvoran, PhD; Miroslav Fikar, PhD; Alojz Mészáros, PhD;

**Assistant Professors:**

Mária Karšaiová, PhD; Magdaléna Ondrovičová; Anna Vasičkaninová; Anna Zemanovičová, PhD;

**PhD students:**

Anton Andrášik; Jozef Dzivák; František Jelenčiak; Michal Kvasnica; Ľubomír Šperka;

**Technical staff:**

Eva Fuseková; Andrea Kalmárová; Anna Širicová; Stanislav Vagač;

### II. TEACHING AND RESEARCH LABORATORIES

**A. Teaching Laboratories:**

Laboratory of Measuring Instruments and Techniques  
Laboratory of Process Control  
Laboratory of Gas Analysis  
Computer Laboratory (PC 486, Pentium)  
Computer Laboratory (LINUX)

**B. Research Laboratories:**

Laboratory of Chemical Reactor Analysis and Control  
Laboratory of Biochemical Process Analysis and Control  
Laboratory of Distillation Column Analysis and Control  
Laboratory of Modelling and Simulation  
Laboratory of Computer Aided Design (Siemens – SIMATIC S-7 300)

### III. TEACHING

**A. Undergraduate Study**

**2nd semester (spring)**

|             |         |                            |
|-------------|---------|----------------------------|
| Informatics | (1-2 h) | Ondrovičová, Vasičkaninová |
|-------------|---------|----------------------------|

**5th semester (autumn)**

|                                |         |  |
|--------------------------------|---------|--|
| Computer Based Data Processing | (0-2 h) | Dzivák, Fikar, Jelenčiak, Karšaiová,<br>Ondrovičová, Vasičkaninová |
|--------------------------------|---------|--|

**6th semester (spring)**

|                                |         |                        |
|--------------------------------|---------|------------------------|
| Automatic Control Fundamentals | (2-0 h) | Bakošová, Danko, Fikar |
|--------------------------------|---------|------------------------|

|  |         |  |
|--|---------|--|
| Laboratory Exercises of Automatic Control Fundamentals | (0-2 h) | Andrašik, Bakošová, Danko, Dzivák, Fikar,<br>Jelenčiak, Karšaiová, Kvasnica, Mészáros,<br>Ondrovičová, Vasičkaninová |
|--|---------|--|

|                   |         |  |
|-------------------|---------|--|
| Bachelor projects | (0-4 h) | Bakošová, Dvoran, Fikar, Mikleš, Ondrovičová,<br>Vasičkaninová |
|-------------------|---------|--|

**7th semester (autumn)**

|                             |         |  |
|-----------------------------|---------|--|
| Process Control             | (1-2 h) | Mészáros   |
| Process Dynamics            | (2-0 h) | Bakošová   |
| Operating Systems           | (1-1 h) | Jelenčiak  |
| Control Devices and Systems | (2-1 h) | Danko  |
| Computer Programs           | (1-2 h) | Vasičkaninová  |
| Laboratory Projects         | (0-8 h) | Bakošová, Danko, Mikleš, Karšaiová,<br>Vasičkaninová |

**8th semester (spring)**

|              |         |        |
|--------------|---------|--------|
| Optimisation | (2-1 h) | Dvoran |
|--------------|---------|--------|

|   |          |  |
|---|----------|--|
| Control Theory I                                  | (2-2 h)  | Karšaiová, Mikleš                                |
| Laboratory Exercises of Control Theory I          | (0-2 h)  | Mikleš   |
| Experimental Identification                       | (2-0 h)  | Fikar  |
| Laboratory Project II                             | (0-6 h)  | Danko, Dvoran, Mészáros                          |
| Modelling and Control of Polymerisation Processes | (2-2 h)  | Dvoran   |
| Process Dynamics                                  | (2-0 h)  | Bakošová   |
| Laboratory Exercises of Process Dynamics          | (0-1 h)  | Bakošová   |
| <b>9th semester (autumn)</b>                      |          |  |
| Control Theory II                                 | (2-0 h)  | Mészáros   |
| Laboratory Exercises of Control Theory II         | (0-2 h)  | Mészáros   |
| Intelligent Control Systems                       | (2-0 h)  | Dvoran   |
| Semestral Project                                 | (0-10 h) | Dvoran, Karšaiová, Mészáros, Mikleš, Ondrovičová |
| CAD Systems                                       | (2-0 h)  | Karšaiová  |
| Industrial Applications of Process Control        | (2-0 h)  | Mikleš   |
| Control of Technological Processes                | (1-2 h)  | Bakošová   |
| <b>10th semester (spring)</b>                     |          |  |
| Diploma Theses                                    |          | Dvoran, Karšaiová, Mészáros                      |
| <b>B. PhD Study</b>                               |          |  |
| Topics in Control Theory                          | (2 h)    | Mikleš   |
| Software and Hardware of Control Systems          | (2 h)    | Danko  |
| Intelligent Control Systems                       | (2 h)    | Dvoran   |
| Modelling and Simulation of Processes             | (2 h)    | Mészáros   |

## IV. CURRENT RESEARCH PROJECTS

### A. Development of advanced control methods for chemical reactors, distillation columns and other plants in chemical and food technology (Ján Mikleš)

The main goals of the project can be formulated in the following items:

To derive mathematical models of chemical and biochemical processes: an exothermic reactor for decomposition of  $H_2O_2$ , a tray distillation column and a stuffed distillation column for separation of binary mixtures, a warm-air drying chamber, a biochemical reactor.

To develop methods and algorithms for system identification: closed-loop identification, identification based on artificial neural network, identification of physical system parameters from measured data.

To investigate modern optimisation methods and algorithms for nonlinear high-order systems, especially for distillation columns and biochemical reactors.

To investigate robust stabilisation and robust feedback control of multivariable systems.

To develop adaptive control methods and adaptive control algorithms for systems of the chemical and food technology.

To include principles of artificial intelligence (expert systems, fuzzy control, neuro-fuzzy control, artificial neural networks) into control structures for chemical processes.

To investigate the predictive control method and to create control algorithms based on the Youla-Kučera parameterisation for solving unconstrained or constrained control problems.

To verify all theoretical results on laboratory models chemical processes.

To transform theoretical and experimental results into industrial conditions and to demonstrate benefits and advantages of advanced process control in chemical and food industry.

The most important results of the project are following:

development of receding horizon iterative dynamic programming with discrete time models,

using Youla-Kučera parameterisation in control design for decoupled control systems,

design of a closed-loop identification method based on the Youla-Kučera parameterisation without model reduction,

pH control in a laboratory fermenter.

### B. Adaptive and intelligent control strategies for processes of chemical/biochemical technology (Alojz Mészáros)

The main goals of the project can be listed as follows:

Design of a new predictive, intelligent control strategy on basis of ANN, (the PID-ANN-P algorithm), and its simulation for linear and non-linear systems.

Design of a new robust, intelligent control strategy on basis of ANN (the PID-ANN-R algorithm), and its simulation for linear and non-linear systems; without as well as in presence of noise and disturbances; without as well as with constraints on control.

Testing the PID-ANN-R procedure on non-linear models of chemical processes.

Design of adaptive  $\lambda$ -tracking control and its verification for non-linear SISO and MIMO systems.

Implementation of control algorithms introduced using ANN (the PID-ANN, PID-ANN-P and PID-ANN-R algorithms) to computer control of laboratory fermenter LF-3; testing performance for real physical circumstances

Implementation of control algorithms derived on basis of  $\lambda$ -tracking policy to direct computer control of laboratory distillation column.

Computer control of laboratory distillation column using adaptive predictive approaches involving low order concentration gradient models.

Selection of the most „successive“ algorithm from the methods proposed and its transformation into software module, suitable for industrial control application.

Original results obtained in the frame of the project are:

adaptive intelligent PID controller with predictive performance,

robust and adaptive controller in terms of neural networks,  
application of adaptive  $\lambda$ -tracking for control of MIMO nonlinear chemical processes – chemical reactor and distillation column.

## V. COOPERATION

### A. Cooperation in Slovakia

Department of Automatic Control Systems, Faculty of Electrical Engineering and Information Technology, Slovak University of Technology, Bratislava

Department of Automation and Control, Faculty of Electrical Engineering and Information Technology, Slovak University of Technology, Bratislava

Department of Automation and Measurement, Faculty of Mechanical Engineering, Slovak University of Technology, Bratislava

Institute of Control Theory and Robotics, Slovak Academy of Sciences, Bratislava

Department of Cybernetics and Artificial Intelligence, Faculty of Electrical Engineering and Informatics, Technical University of Košice, Košice

Department of Management and Control Engineering, BERG Faculty, Technical University of Košice, Košice

Slovnaft, Inc., Bratislava

NCHZ, Inc., Nováky

ProCS, Ltd., Šaľa

### B. International Cooperation

Department of Process Control and Computer Techniques, Faculty of Chemical Technology, University of Pardubice, Pardubice, Czech Republic

- Control system design

Department of Computing and Control Engineering, Institute of Chemical Technology, Prague, Czech Republic

- Control of bioreactors

Department of Control Theory, Institute of Information Technologies, Tomas Bata University, Zlín, Czech Republic

- Adaptive control

- Robust control

Institute of Information Theory and Automation of the Academy of Sciences of the Czech Republic, Prague, Czech Republic

- Adaptive control

- Predictive control

Trnka Laboratory for Automatic Control, Faculty of Electrical Engineering, Czech Technical University, Prague, Czech Republic

- Adaptive control

- Predictive control

LSGC-CNRS, Ecole Nationale Supérieure des Industries Chimiques (ENSIC), Nancy, France

- Dynamic optimisation of distillation columns

- Control of distillation columns

Ecole Nationale Supérieure des Ingénieurs de Génie Chimique-Chemin de la Loge (ENSIGC), Toulouse, France

- Neural networks

- Predictive control

Ruhr University, Bochum, Germany

- Closed-loop identification

- Predictive control

Technical University of Budapest, Budapest, Hungary

- Modelling of chemical processes

Technical University of Vienna, Vienna, Austria,

- Optimisation of combustion processes

### C. Membership in Domestic Organisations and Societies

Slovak Society of Cybernetics and Informatics,  
Bratislava

A. Mészáros, J. Mikleš

Slovak Society of Chemical Engineering, Bratislava

M. Bakošová, J. Danko, J. Dvoran, M. Fikar, M. Karšaiová, A. Mészáros, J. Mikleš, M. Ondrovičová, A. Zemanovičová

Slovak Union of Industrial Chemistry,  
Science-Technical Society, Bratislava

M. Bakošová, J. Danko, J. Dvoran, M. Fikar, M. Karšaiová, A. Mészáros, J. Mikleš, M. Ondrovičová, A. Vasičkaninová, A. Zemanovičová

### D. Membership in International Organisations and Societies

International Federation of Automatic Control, Laxenburg,  
Austria

J. Mikleš

European Federation of Biotechnology, Brussels, Belgium

A. Mészáros

The New York Academy of Sciences, New York, USA

A. Mészáros

### E. International Scientific Programmes

#### 1. INCO COPERNICUS

No. CP97:7010, The European Network for Industrial Application of Polynomial Design Methods – EUROPOLY

Coordinator at the FCFT STU: J. Mikleš

Coordinator of the project: Czech University of Technology, Prague, Czech Republic;

Participants: Institute of Information Theory and Automation of the Academy of Sciences of the Czech Republic, Prague, Czech Republic; University of Twente, Twente, Netherlands; University of Glasgow, Glasgow, Great Britain; Uppsala University, Uppsala,

Sweden; University of Strathclyde, Strathclyde, Great Britain; Politecnico di Milano, Milan, Italy; CNRS – LAAS, Toulouse, France; Tomas Bata University, Zlín, Czech Republic; Department of Information Engineering and Process Control, Faculty of Chemical and Food Technology, Slovak University of Technology, Bratislava, Slovakia; Warsaw University of Technology, Warsaw, Poland; Swiss Federal Institute of Technology, Zurich, Switzerland; ProCS, Ltd., Šaľa, Slovakia; Compureg Plzeň, Plzeň, Czech Republic; Period: January 1998 – December 2001

#### 2. LEONARDO

No. RO/00/B/F/PP141028, Eurocompetencies Transfer in Vocational Guidance for Young Specialists in Bioscience Field

Coordinator at the FCFT STU: V. Báleš

Coordinator of the project: Ost European Centrum, University Hohenheim, Germany;

Participants: Ost European Centrum, University Hohenheim, Germany; Romanian Society of Biotechnology and Bioengineering, Bucharest, Romania; Research Institute for Chemistry, Bucharest, Romania; University Politehnica, Bucharest, Romania; Pluri Consultants SRL, Bucharest, Romania; University of Agronomic Sciences and Veterinary Medicine, Bucharest, Romania; CERA Foundation, Bucharest, Romania; Department of Chemical and Biochemical Engineering, Faculty of Chemical and Food Technology, Slovak University of Technology, Bratislava, Slovakia; Department of Information Engineering and Process Control, Faculty of Chemical and Food Technology, Slovak University of Technology, Bratislava, Slovakia; Natural Resources Institute, University of Greenwich, Greenwich, Great Britain

Period: November 2000 – November 2003

#### 3. Project of Austrian - Slovak Scientific Cooperation: Aktion Österreich – Slowakei

No. 26s12, Optimierung des Verbrennungsprozess von dem Standpunkt des Umweltschutzes (Optimisation of a Combustion Process from the Environmental Point of View)

Coordinator at the FCFT STU: A. Zemanovičová

Coordinator of the project: Technical University of Vienna, Vienna, Austria

Participants: Department of Information Engineering and Process Control, Faculty of Chemical and Food Technology, Slovak University of Technology, Bratislava, Slovakia; Technical University of Vienna, Vienna, Austria

Period: April 1999 – December 2001

#### 4. Project of Slovak – Czech Scientific Cooperation

No. 112/344 Rozvoj metód moderného riadenia procesov chemickej a potravinárskej technológie (Development of Advanced Control Methods for Processes of Chemical and Food Technology)

Coordinator at the FCFT STU: J. Mikleš

Participants: Department of Information Engineering and Process Control, Faculty of Chemical and Food Technology, Bratislava, Slovakia; Department of Process Control and Computer Techniques, University of Pardubice, Pardubice, Czech Republic

Period: January 2000 – December 2001

### F. Visitors from Abroad

Prof. P. Dostál

Tomas Bata University, Zlín, Czech Republic, June 2001 (1 day)

F. Dušek, PhD

University of Pardubice, Czech Republic, June 2001 (3 days)

D. Honc

University of Pardubice, Czech Republic, June 2001 (3 days)

J. Macháček, PhD

University of Pardubice, Czech Republic, June 2001 (3 days)

Prof. I. Taufer

University of Pardubice, Czech Republic, March 2001 (2 days)

Prof. I. Taufer

University of Pardubice, Czech Republic, June 2001 (2 days)

Prof. I. Taufer

University of Pardubice, Czech Republic, November 2001 (4 days)

### G. Visits of Staff Members and PhD Students to Foreign Institutions

A. Andrášik

University of Pardubice, Pardubice, Czech Republic, November 2001 (4 days)

M. Bakošová

Tomas Bata University, Zlín, Czech Republic, June 2001 (2 days)

M. Bakošová

University of Pardubice, Czech Republic, September 2001 (3 days)

M. Bakošová

Conference Information Engineering and Control, Prague, Czech Republic, September 4, 2001

M. Bakošová

University of Pardubice, Czech Republic, November 2001 (2 days)

J. Dvoran

Conference Information Engineering and Control, Prague, Czech Republic, September 4, 2001

M. Fikar

ENSIC, Nancy, France, July 2001 (24 days)

M. Fikar

ENSIC, Nancy, France, September - December 2001 (4 months)

M. Kvasnica

ENSIGC, Toulouse, France, July 2001 (14 days)

A. Mészáros

Technical University of Budapest, Hungary, January, 2001 (2 days)

A. Mészáros

Technical University of Bucharest, Romania, June 2001 (5 days)

A. Mészáros

World MultiConference on Systemics, Cybernetics and Informatics, Orlando, USA, July 22-25, 2001

A. Mészáros

Technical University of Budapest, Hungary, September, 2001 (2 days)

A. Mészáros

Technical University of Budapest, Hungary, October, 2001 (1 day)

A. Mészáros

Tomas Bata University, Zlín, Czech Republic, October 2001 (2 days)

A. Mészáros

University Hohenheim, Stuttgart, Germany, November 2001 (6 days)

J. Mikleš

European Control Conference, Porto, Portugal, September 3 – 7, 2001

J. Mikleš

Ruhr University, Bochum, Germany, July 2001 (25 days)

J. Mikleš

University Erlangen, Nurnburg, Germany, August 2001 (4 days)

M. Ondrovičová

University of Pardubice, Czech Republic, September 2001 (3 days)

M. Ondrovičová

University of Pardubice, Czech Republic, November 2001 (2 days)

A. Vasičkaninová

Technical University of Vienna, Austria, October 2001 (5 days)

|                  |   |
|------------------|---|
| A. Vasičkaninová | University of Pardubice, Czech Republic, November 2001 (2 days) |
| A. Zemanovičová  | Technical University of Vienna, Austria, February 2001 (1 day)  |
| A. Zemanovičová  | Technical University of Vienna, Austria, June 2001 (2 days)     |
| A. Zemanovičová  | Technical University of Vienna, Austria, August 2001 (22 days)  |
| A. Zemanovičová  | Technical University of Vienna, Austria, September 2001 (1 day) |
| A. Zemanovičová  | Technical University of Vienna, Austria, October 2001 (1 day)   |
| A. Zemanovičová  | Technical University of Vienna, Austria, November 2001 (1 day)  |
| A. Zemanovičová  | University of Pardubice, Czech Republic, November 2001 (2 days) |
| A. Zemanovičová  | Technical University of Vienna, Austria, December 2001 (1 day)  |

## VI. THESES AND DISSERTATIONS

### A. Graduate Theses (MS Degree) for state examinations after five years of study (supervisors are written in brackets)

|                |   |
|----------------|---|
| Dutková I.:    | Identification and control of laboratory fermenter LF3. (A. Mészáros)             |
| Nikodémová L.: | Testing of an optimisation toolbox in MATLAB environment (J. Dvoran)              |
| Skurková M.:   | Decentralised control of a tray distillation column. (M. Karšaiová)               |
| Tallo M.:      | Neuro-fuzzy based control system for a technological process. (J. Dvoran)         |
| Jankovčin J.:  | Optimisation and control of a chemical reactor. (M. Karšaiová)                    |
| Majerník P.:   | Application of PLC and SCADA systems for control of real processes. (A. Mészáros) |
| Šperka L.:     | Artificial neural network based system identification and control. (A. Mészáros)  |

## VII. PUBLICATIONS

### A. Journals (\*registered in Current Contents)

- [1] Andrášik A., Mészáros A., Šperka L.: Adaptívne inteligentné PID riadenie v prediktívnom zmysle. Adaptive intelligent PID control in predictive form (in Slovak). AT&P Journal 8 (plus1), 39 – 41 (2001).
- [2] Andrášik A., Mészáros A.: Riadenie pH v laboratórnom fermentore LF-3. Control of pH in laboratory fermenter LF-3 (in Slovak). AT&P Journal 8 (4), 63 – 64 (2001).
- [3] Bakošová M., Ondrovičová M., Dvoran J., Debnárová L.: Riadenie rektifikačnej kolóny. Control of a distillation column (in Slovak). AT&P Journal 8 (11), 52 – 53 (2001).
- [4] Dvoran J., Hudáček P.: Simulačné overenie hybridného neuro-fuzzy riadiaceho systému. Verifying of a hybrid neuro-fuzzy control system by simulations (in Slovak). AT&P Journal 8 (plus1), 18 – 21 (2001).
- [5] Mészáros A.: Niektoré otázky riadenia procesov biochemickej technológie. Some aspects of control of biochemical processes (in Slovak). AT&P Journal 8 (4), 60 – 62 (2001).
- [6] Mikleš J., Čirka L., Fikar M.: Adaptívne LQ riadenie CSTR s využitím YK parametrizácie regulátora a modelu objektu. Adaptive LQ control of a CSTR using YK parameterisation of a controller and a process model (in Slovak). AT&P Journal 8 (11), 57 – 59 (2001).
- [7]\* Rusnák A., Fikar M., Latifi M. A., Mészáros A.: Receding Horizon Iterative Dynamic Programming with Discrete Time Models. Computers Chem. Engng. 25 (1), 161-167 (2001).
- [8] Zemanovičová A.: Spalovací proces. AT&P Journal 8 (4), 65 – 67 (2001).

### B. Conferences (\*international conferences)

- [1]\* Andrášik A., Mészáros A.: Identification and computer control of a laboratory fermenter. In: Proc. 13. Int. Conf. Process Control'01. Štrbské Pleso, High Tatras (Slovakia), June 11-14, 2001. KIRP CHTF STU Bratislava, CD ROM 302 (2001).
- [2]\* Bachmann G., Hofbauer H., Zemanovičová A., Vasičkaninová A.: Determination of the calorific value of heterogeneous materials in a multi-kilogram capacity calorimeter. In: CD ROM of the 40<sup>th</sup> Int. Petroleum Conf.. Bratislava (Slovakia), Sept. 17-19, 2001. Slovnaft, Inc., Bratislava, CD ROM P-G-57.
- [3]\* Bakošová M., Dvoran, J.: Laboratory of real processes at the DPC FCFE STU Bratislava. In: Proceedings of the Conf. Information Engineering and Control. Prague (Czech Republic), September 4, 2001. Masaryk Academy of Work, Prague, pp. 87–88 (2001).
- [4]\* Bakošová M., Mészáros A., Ondrovičová M., Karšaiová M.: Application of adaptive  $\lambda$ -tracking for control of MIMO nonlinear chemical processes. In: CD ROM of full texts of the 28<sup>th</sup> Int. Conf. of SSCHE. Tatranské Matliare (Slovakia), May 21–25, 2001. SSCHE Bratislava, CD ROM P123 (2001).
- [5]\* Bakošová M., Mészáros A., Ondrovičová M., Karšaiová M.: Application of adaptive  $\lambda$ -tracking for control of MIMO nonlinear chemical processes. In: Proceedings of the 28<sup>th</sup> Int. Conf. of SSCHE. Tatranské Matliare (Slovakia), May 21–25, 2001. STU Bratislava, p. 121 (2001).
- [6]\* Bakošová M., Mészáros A.: Decentralized Adaptive Control of Distillation Columns - A Case Study. In: Proc. World MultiConf. on Systemics, Cybernetics and Informatics SCI 2001. Orlando (USA), July 22-25, 2001. Int. Institute of Informatics and Systemics, Orlando, p. 563-568 (2001).
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- [9]\* Čírka L., Fikar M., Mikleš J.: A deterministic LQ tracking problem: Parametrisation of the controller and the plant. In: Proc. 13. Int. Conf. Process Control'01. Štrbské Pleso, High Tatras (Slovakia), June 11-14, 2001. KIRP CHTF STU Bratislava, CD ROM 304 (2001).
- [10]\* Čírka L., Fikar M., Mikleš J.: A deterministic LQ tracking problem: Parametrisation of the controller and the plant. In: CDROM Medzinárodnej konferencie SSKI Kybernetika a informatika. Piešťany (Slovakia), April 5-6, 2001. SSKI Bratislava, CD ROM (2001).
- [11]\* Čírka L., Fikar M., Mikleš J.: A deterministic LQ tracking problem: Parametrisation of the controller and the plant. In: Summaries Volume of the 13. Int. Conf. Process Control'01. Štrbské Pleso, High Tatras (Slovakia), June 11-14, 2001. Slovak University of Technology Bratislava, Slovak Republic. p. 237 (2001).
- [12]\* Čírka L., Fikar M., Mikleš J.: A deterministic LQ tracking problem: Parametrisation of the controller and the plant. In: Zborník abstraktov Medzinárodnej konferencie SSKI Kybernetika a informatika. Piešťany (Slovakia), April 5-6, 2001. SSKI Bratislava, pp. 142-143 (2001).
- [13]\* Čírka L., Mikleš J., Fikar M.: A deterministic LQ tracking problem: Parametrisation of the controller. In: Proc. 13. Int. Conf. Process Control'01. Štrbské Pleso, High Tatras (Slovakia), June 11-14, 2001. KIRP CHTF STU Bratislava, CD ROM 303 (2001).
- [14]\* Čírka L., Mikleš J., Fikar M.: A deterministic LQ tracking problem: Parametrisation of the controller. In: Summaries Volume of the 13. Int. Conf. Process Control'01. Štrbské Pleso, High Tatras (Slovakia), June 11-14, 2001. Slovak University of Technology Bratislava, Slovak Republic. p. 236 (2001).
- [15]\* Danko J., Ondrovičová M.: An approach to the control of a laboratory tank system. In: Proc. 13. Int. Conf. Process Control'01. Štrbské Pleso, High Tatras (Slovakia), June 11-14, 2001. KIRP CHTF STU Bratislava, CD ROM 319 (2001).
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- [22]\* Jelenčiak F., Mikleš J.: Process identification: Nonlinear systems. In: Proc. 13. Int. Conf. Process Control'01. Štrbské Pleso, High Tatras (Slovakia), June 11-14, 2001. KIRP CHTF STU Bratislava, CD ROM 311 (2001).
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- [24]\* Karšaiová M., Bakošová M., Ondrovičová M.: Control of Distillation Columns. In: Proc. 13. Int. Conf. Process Control'01. Štrbské Pleso, High Tatras (Slovakia), June 11-14, 2001. KIRP CHTF STU Bratislava, CD ROM 318 (2001).
- [25]\* Karšaiová M., Bakošová M., Ondrovičová M.: Control of Distillation Columns. In: Summaries Volume of the 13. Int. Conf. Process Control'01. Štrbské Pleso, High Tatras (Slovakia), June 11-14, 2001. Slovak University of Technology Bratislava, Slovak Republic. p. 215 (2001).
- [26]\* Kožka Š., Mikleš J., Fikar M.: The Youla-Kucera parameterisation: Standard and modified identification algorithm. In: Proc. Int. Carpathian Control Conf. ICCS 2001. Krynica (Poland), May 22-25, 2001. AGH Krakow, pp.183-188 (2001).
- [27]\* Kožka Š., Mikleš J.: An identification based on the Youla-Kucera parameterisation without model reduction. In: Proceedings of the 13. Int. Conf. Process Control'01. Štrbské Pleso, High Tatras (Slovakia), June 11-14, 2001. KIRP CHTF STU Bratislava, CD ROM 308 (2001).
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- [29]\* Kožka Š., Zemanovičová A., Hofbauer H., Bachmann G.: Identification of the experimental multi-kilogram capacity calorimeter. In: Proceedings of the 13. Int. Conf. Process Control'01. Štrbské Pleso, High Tatras (Slovakia), June 11-14, 2001. KIRP CHTF STU Bratislava, CD ROM 307 (2001).
- [30]\* Kožka Š., Zemanovičová A., Hofbauer H., Bachmann G.: Identification of the experimental multi-kilogram capacity calorimeter. In: Summaries Volume of the 13. Int. Conf. Process Control'01. Štrbské Pleso, High Tatras (Slovakia), June 11-14, 2001. Slovak University of Technology Bratislava, Slovak Republic. p. 79 (2001).
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- of Technology Bratislava, Slovak Republic. p. 147 (2001).
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- [38] Kvasnica M., Kožka Š., Mikleš J.: Využitie riadiaceho automatu Simatic S7-300 pri riadení laboratórneho reaktora. . Using of a PLC Simatic S7-300 for control of a laboratory reactor (in Slovak). In: Zborník abstraktov Medzinárodnej konferencie SSKI Kybernetika a informatika. Piešťany (Slovakia), April 5–6, 2001. SSKI Bratislava, pp. 91 – 92 (2001).
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- [41]\* Mészáros A., Andrášik A.: Adaptive intelligent PID control with predictive performance. In: Proc. World MultiConf. on Systemics, Cybernetics and Informatics SCI 2001. Orlando (USA), July 22-25, 2001. Int. Institute of Informatics and Systemics, Orlando, pp. 569 – 574 (2001).
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### C. Technical Reports

- [1] Fikar M.: Dynamic Optimisation of Small-size Wastewater Treatment Plants. Technical report. Laboratoire des Sciences du Genie Chimique, CNRS, Nancy, France, 2001.

## DEPARTMENT OF SACCHARIDES AND FOOD PRESERVATION

**Head of the Department:**  
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### I. STAFF

**Full Professors:**

Alexander Dandár, PhD,DSc; Alexander Pribela, PhD,DSc

**Associate Professors:**

Ladislav Dodok, PhD; Jolana Karovičová PhD; Mária Takácsová,PhD;

**Assistant Professors:**

Alica Burisová; Gabriel Greif; Eva Hybenová, PhD; Mária Kováčová, PhD; Ladislav Staruch, PhD; Soňa Škrovánková

**Research Fellows:**

Viola Buchtová; Marta Kostičová; Zuzana Smelíková, PhD; Anna Stahelová

**PhD Students:**

Silvia Grochalová; Zlatica Kohajdová; Drahomíra Lukáčová; Kitti Németh

**Technical Staff:**

Žofia Fórová; Katarína Halasová; Jarmila Mikletičová; Helena Morávková; Gabriela Sisáková; Eva Vosátková

### II. TEACHING AND RESEARCH LABORATORIES

Laboratory of Sugar Technology  
Laboratory of Starch Chemistry and Technology  
Laboratory of Cereal Technology  
Laboratory of Canned Products  
Laboratory of Meat and Meat Products  
Laboratory of Microbiology  
Sensory Laboratory  
Laboratory of Food Chemistry and Analysis  
Laboratory of Food Preservation  
Laboratory of Separation Methods

### III. TEACHING

#### A. Undergraduate Study

**5th semester (autumn)**

|                                 |           |            |
|---------------------------------|-----------|------------|
| Food Chemistry                  | (2-0-0 h) | Takácsová  |
| Fundamentals of Food Technology | (2-0-0 h) | Karovičová |

**6th semester (spring)**

|                             |           |          |
|-----------------------------|-----------|----------|
| Food Analysis               | (2-0-0 h) | Kováčová |
| Laboratory of Food Analysis | (0-0-4 h) | Kováčová |

**7th semester (autumn)**

|   |           |          |
|---|-----------|----------|
| Chemistry and Technology of Saccharides | (2-2-0 h) | Burisová |
| Theory of Food Preservation             | (3-1-0 h) | Greif    |
| Semestral Project                       | (0-0-5)   |          |
| Food Foreign Substances                 | (2-0-0 h) | Hybenová |

**8th semester (spring)**

|                                      |           |                     |
|--------------------------------------|-----------|---------------------|
| Cereal Chemistry and Technology      | (4-1-0 h) | Dodok               |
| Sugar Technology                     | (4-0-0 h) | Dandár              |
| Food Chemistry II                    | (2-0-0 h) | Takácsová           |
| Laboratory of the Specialization I.  | (0-0-5 h) |                     |
| Preserved and Frozen Food Technology | (2-1-0 h) | Karovičová          |
| Meat and Poultry Technology          | (2-1-0 h) | Staruch             |
| Raw Materials for Canning Industry   | (2-0-0 h) | Karovičová, Staruch |
| Semestral Project                    | (0-0-5)   |                     |

**9 th semester (autumn)**

|  |           |                      |
|--|-----------|----------------------|
| Food Evaluation  | (2-0-2 h) | Pribela, Škrovánková |
| Chemical Engineering Processes<br>in Saccharide Technology | (2-0-0 h) | Dandár               |
| Technology Optimizing in Canning Industry                  | (1-1-0 h) | Greif                |

|                                      |            |                          |
|--------------------------------------|------------|--------------------------|
| Laboratory of the Specialization II. | (0-0-4 h)  |                          |
| Electives:                           |            |                          |
| Optimizing of Sugar Technology       | (2-0-0 h)  | Dandár                   |
| Food Analysis II                     | (2-0-2 h)  | Prachár                  |
| Meat and Poultry Technology II       | (2-0-0 h)  | Staruch                  |
| <b>10th semester (spring)</b>        |            |                          |
| Diploma Thesis                       | (0-0-27 h) | all members of the staff |

#### IV. CURRENT RESEARCH PROJECTS

##### A. Optimizing of physicochemical and biological effects with respect to increase of nutritive and sensory value of foodstuffs (Alexander Dandár)

Physicochemical properties of amaranth starches were studied. On the basis of our results the starches mentioned above will be used in pharmaceutical industry too. Technological proposal for production of new cereal products (cereal mixtures ) with higher nutritive value was submitted.

The data for production of food supplements with glucan of the highest quality were worked out. Clinical tests with oncological patients were made. Natural food additives ( cereal and pseudocereal starches and legume starch ) were added into selected food products to increase their nutritive value, sensory properties and durability.

Suitable methods for determination of antioxidative effects of natural substances were tested. The kinetics of colorant formation in the process of liming of raw juice was evaluated. Effect of temperature, amount of lime milk, amino acids and reducing sugars concentration on colorants formation was analysed.

Natural additives ( ascorbic acid, alfa-tocopherol acetate, bacteriocins, starters combined with mould ) into fermented meat products to increase their durability and sensory properties were tested.

##### B. Bioconservation of plant and animal raw materials using probiotic bacteria of human health promoters to eliminate the food contaminants and to increase the nutritive value of food products (Jolana Karovičová)

Isolation and identification of lactic acid bacteria and their selection on the basis of lactic and acetic acids production were studied. The changes of nitrates and nitrites concentration and the production of free amino acids and biogenic amines in selected plant substrates were analysed. Probiotic properties of selected strains of *Lactobacillus* for example survival at low pH value and the production of bacteriocins and their growth in selected substrates were studied. Sensory evaluation of lactic fermented vegetables as well as vegetable juices was made. This evaluation was realized by group of specialists using the profile method. The results of sensory and analytical methods were evaluated by PCA method. Lactic bacteria of *Enterobacter aerogenes* were analysed under different conditions ( different concentration of glucose, potassium sorbate, sodium benzoate, NaCl ) Their growth and production of metabolite on synthetic substrates (MPB, GTK) and on natural one (cabbage juice) at different temperature were observed. Validity parameters of organic acids by capillary ITP were defined.

#### V. COOPERATION

##### A. Cooperation in Slovakia

Ministry of Agriculture of Slovak Republic, Bratislava  
 Institute of Food Research, Bratislava  
 Slovak Academy of Sciences, Bratislava  
 Považský cukrovar Co, Trenčianska Teplá  
 Slovak Sugar Technology Association, Bratislava  
 OLD HEROLD Co, Trenčín  
 SLOVAMYL Ltd, Bratislava  
 Mäsozávod, Bratislava  
 University of Agriculture, Nitra  
 ADIPO Ltd, Nitra

##### B. International Cooperation

Institute of Food Research, Prague, Czech Republic  
 College of Agriculture, Brno, Czech Republic  
 Škrobárny Co, Brno, Czech Republic  
 Institute of Chemical Technology, Prague, Czech Republic  
 Institute of Food Research, Manchester, UK  
 Akademia Ekonomiczna, Wrocław, Poland  
 Technical University, Berlin, Germany  
 Technical University, Lodž, Poland

##### C. Membership in Domestic Organizations and Societies

Slovak Society of Agricultural, Food and Forestry Sciences, Bratislava (A. Dandár, M. Takáčsová, L.Staruch )  
 Slovak Academy of Agricultural Sciences, Bratislava (A.Dandár, L.Dodok)  
 Slovak Academy of Technical Sciences, Bratislava (A.Dandár)  
 Foundation "SLOVAK GOLD", Bratislava (L.Staruch)  
 Slovak Institute of Technical Normalization, Bratislava ( L.Dodok, L.Staruch)

The Union of Slovak Butchers, Bratislava (L. Staruch)  
 Slovak National Committee of International  
 Commission for Uniform Methods of Sugar Analysis  
 - ICUMSA (A. Dandár)  
 Slovak Agricultural Academy, Nitra (A. Pribela, A. Dandár, L. Dodok)

#### D. Membership in International Organizations and Societies:

International Commission for Uniform Methods  
 of Sugar Analysis - ICUMSA, Italy (A. Dandár)  
 American Chemical Society (A. Dandár)  
 Commission International Technique de Sucrierie  
 - CITS, Brussels, Belgium (A. Dandár)  
 Verein der Zuckerfabriken Österreichs,  
 Vienna, Austria (A. Dandár)  
 Stowarzyszenie Techników Cukrowników,  
 Wrocław, Poland (A. Dandár)  
 WEPASA – World Poultry Scientific Association,  
 Israel (L. Staruch)

#### F. International Scientific Programmes:

SOCRATES/ERASMUS  
 a/ 55792-CP-1-98-FR-ERASMUS-ETN, /FOODNET-Food Studies in Europe  
 A. Dandár – FCHFT STU, ENSIA, Massy Cedex, France

#### H. Visits of Staff Members and PhD Students to Foreign Institutions

A. Dandár, Takácsová Technical University Krakow, Poland, June 2001 (4 days)  
 A. Dandár Commission International Technique de Sucrierie - CITS, Brussels,  
 Belgium, February 2001 (3 days)  
 A. Dandár Zuckerfabrik Hohenau, Austria, November 2001 (2 days)

## VI. THESES AND DISSERTATIONS

### A. Graduate Theses (MS Degree) for state examinations after 5 years of study (supervisors are written in brackets)

Bunová J.: Study of pectic substances – new pectic esters. (E. Malovíková)  
 Dziváková – Horváthová E.: Study of flow properties in cereal starch and meal after addition of  
 different xylanes. (A. Burisová)  
 Džupová A.: Modern trends in bread production. (L. Dodok)  
 Golasová K.: Effect of the components of pectin jelly on its properties. (A. Burisová)  
 Grochalová S.: Study of the stability and antioxidative effects of flavonoids in onion.  
 (M. Kováčová)  
 Chomová – Lojová L.: Study of amino acids in spices. (V. Buchtová)  
 Kubová A.: Effect of NaCl concentration and pH value on the growth of  
*Enterococcus faecium* and on tyramine production (G. Greif)  
 Krahulcová - Guľáková J.: Analysis of lactic fermented products. (Z. Kohajdová)  
 Lukačová D.: Determination of selected metabolites of microorganisms by capillary  
 isotachopheresis. (J. Karovičová)  
 Mikušincová - Ďurinová N.: Determination of vitamin B12 in vegetarian food. (E. Hybenová)  
 Moskaľová M.: Use of lactic acid in meat industry. (L. Staruch)  
 Pavláková B.: Separation of non-starch polysaccharides from pseudocereals and  
 effect of hemicellulose on properties of dough. (Z. Hromádková)  
 Šiška R.: Effect of improvers on rheological properties of dough and of final  
 product (L. Dodok)  
 Uličná K.: Determination of microbial activity by MICROZYM – L analyser during  
 saccharose extraction. (A. Dandár)  
 Vadovič P.: Effect of natural antioxidants on stability of lipids. (M. Takácsová)

## VII. PUBLICATIONS

### A. Journals (\*registered in Current Contents)

- [1]\* Burisová A., Dodok L., Škrovánková S., Serulová D.: The influence of substitution of wheat flour by amaranth flour on fermentative gas production and quality of bread. *Rostlinná výroba* 47, 2001, p. 276-279.
- [2]\* Burisová A., Tomášková B., Sasinková V., Ebringerová A.: Isolation and characterization of the non-starch polysaccharides of amaranth seed. *Chemical Papers*, 55, 2001, p. 254-260.
- [3] Burisová, A.-Dodok, L.: Objavte zlato lnkov. *Zdravie*, č. 8, 2001, s. 16-17.
- [4]\* Dandár, A., Kopecký, J., Uličná, K.: Stanovenie stupňa mikrobiálnej kontaminácie pri extrakcii sacharózy pomocou analyzátoru MICROZYM – L. Determination of bacterial contamination during extraction of saccharose by MICROZYM – L analyser (in Slovak). *Listy cukrov. a řep.* 117, 2001, 192-193.
- [5]\* Dang, M.N., Takácsová, M., Nguyen, D.V., Kristianová, K.: Antioxidant activity of essential oils from various spices. *Nahrung*

- 45, 2001, p.64-66.
- [6] Karovičová J., Greif G., Kohajdová Z., Hybenová E.: Využitie multivariačnej analýzy pri hodnotení mliečne fermentovaných zeleninových štiav. Application of multivariate analysis in evaluation of fermented vegetable juices (in Slovak). Bull Food Res. 40(2), 119-131 (2001).
- [7] Karovičová J.: Biogénne amíny-vznik, metódy stanovenia a výskyt v potravinách. Biogenic amines – formation, methods of determination and its presence in foods (in Slovak). Bull Food Res. 40(2), 75-89 (2001).
- [8] Kohajdová,Z., Karovičová,J.: Biogénne amíny-vznik, metódy stanovenia a výskyt v potravinách. Bull Food Res. 40(2), 75-89 (2001)
- [9] Staruch, L. - Strmiska, F.: Využitie štartovacích kultúr v mäsovom priemysle. Starters application in meat industry (in Slovak). Výživa a zdravie, 46, 2001, s. 17 - 20.
- [10] Staruch, L., Staruchová, M., Kajaba, I., Strmiska, F.: Hovädzie mäso. Beef (in Slovak). Výživa a zdravie, 46, 2001, s. 58 – 62.
- [11]\* Uličná, K., Dandár, A., Kopecský, J., Fabián, A., Paulenová, L.: Použitie prípravkov typu SUCAZUR v cukrovarníctve. Using of SUCAZUR in sugar technology (in Slovak). Listy cukrov. a řep 117, 2001, 156-159.

## B. Conferences (\*international conferences)

- [1]\* Dodok L., Buchtová V., Hozová B., Staruch L., Burisová A.: Vplyv zlepšujúcich prípravkov na reologické vlastnosti ciest. Effect of improvers on rheological properties of the dough ( in Slovak ).In: Proceedings of the 32nd Symposia „New Trends of Food Production and Evaluation“, Skalský Dvůr, Czech Republic, May 28. - 30. 2001, p. 47
- [2]\* Buchtová, V., Staruch, L., Dodok, L., Chomová, L.: Štúdium koncentrácie aminokyselín v korení. Study of amino acids concentration in spices (in Slovak). In: Proceedings of the 32nd Symposia „New Trends of Food Production and Evaluation“, Skalský Dvůr, Czech Republic, May 28. - 30. 2001, p. 51
- [3]\* Staruch, L., Chalupka, B., Sirotná, Z., Heriban, L.: Kyselina mliečna a jej uplatnenie pri dekontaminácii jatočných tiel. Application of lactic acid in the process of decontamination of slaughterhouse animals (in Slovak). In: Proceedings of the 32nd Symposia „New Trends of Food Production and Evaluation“, Skalský Dvůr, Czech Republic, May 28. - 30. 2001, p. 52
- [4]\* Kováčová, M., Takáčsová,M., Gajdoštinová, N.: Faktory vplyvajúce na stabilitu flavonoidov. Some factors which have the influence on the stability of flavonoids (in Slovak).In: Proceedings of the 32nd Symposia „New Trends of Food Production and Evaluation“, Skalský Dvůr, Czech Republic, May 28. - 30. 2001, p.27-28
- [5]\* Németh, K., Takáčsová, M., Stahelová, A., Hencz, M., Staruch, L.: Application of Cereals for Rapessed Oil Stabilisation. International Conference of Young Scientists Tavazsi Szél 2001, April 20.-22.4.2001, Szent István Egyetem Gödöllő, Hungary (lecture)
- [6] Buchtová, V.,Dodok, L., Chalupka, B.: Štúdium obsahu aminokyselín v jemnom trvanlivom pečive. Study of amino acids content in bisquits (in Slovak). In: Proceedings of the XIII th International Conference LABORALIM 2001, B. Bystrica, Slovak Republic, February 7.-8. 2001, p.78-81
- [7] Dandár, A., Kopecský, J., Uličná K.: Stanovenie stupňa kontaminácie v extraktore pomocou prístroja MIKROZYL-M. Determination of the degree of contamination in extractor by MIKROZYL –M (in Slovak). In: :Proceedings of the XIII th International Conference LABORALIM 2001, B. Bystrica, Slovak Republic, February 7.-8. 2001, p.41-47
- [8] Uličná, K., Dandár, A., Kopecský, J., Fabián, J., Paulenová, L.: Výsledky meraní mikrobiálnej kontaminácie s použitím biocídu SUCAZUR v prevádzke cukrovaru. The measurement of microbial contamination in sugar factory by biocide SUCAZUR (in Slovak). In.: Proceedings of the XIII th International Conference LABORALIM 2001, B. Bystrica, Slovak Republic, February 7.-8. 2001, p.256-260
- [9] Staruch,L., Chalupka,B., Sirotná,Z., Heriban, L.: Dekontaminácia povrchu jatočných tiel aplikáciou kyseliny mliečnej. Decontamination of slaughterhouse animals by lactic acid (in Slovak). In.: Proceedings of the XIII th International Conference LABORALIM 2001, B. Bystrica, Slovak Republic, February 7.-8. 2001, p.226-235
- [10] Ondrejka, J. - Staruch, L.:Nutnosť aplikácie systému HACCP v spoločnom stravovaní. Application of HACCP in communal eating (in Slovak). In: Proceedings of the XIII th International Conference LABORALIM 2001, B. Bystrica, Slovak Republic, February 7.-8. 2001, p. 261-267
- [11] Šoltýsová, J. Staruch, L.:Význam a kontrola polyfosfátov v potravinách.Importance and control of polyphosphates in foods (in Slovak). In: Proceedings of the XIII th International Conference LABORALIM 2001, B. Bystrica, Slovak Republic, February 7.-8. 2001, p. 311-314
- [12] Golian, J. Pavelka, M. Staruch, L.: Zhodnotenie obsahu vybraných chemických prvkov v mäsových výrobkoch. Evaluation of selected chemical elements in meat products (in Slovak). In: Proceedings of the XIII th International Conference LABORALIM 2001, B. Bystrica, Slovak Republic, February 7.-8. 2001, p. 346-349
- [13] Škrovánková, S.-Takáčsová, M.-Magdolenová, C.: Senzorické hodnotenie horkej chuti červených vín I. Sensory analysis of bitter taste in red wine I (in Slovak). In: Proceedings of the XIII th International Conference LABORALIM 2001, B. Bystrica, Slovak Republic, February 7.-8. 2001, p. 241-244
- [14] Škrovánková, S.-Takáčsová, M.-Magdolenová, C.: Senzorické hodnotenie horkej chuti červených vín II. Sensory analysis of bitter taste in red wine II (in Slovak). In: Proceedings of the XIII th International Conference LABORALIM 2001, B. Bystrica, Slovak Republic, February 7.-8. 2001, p. 245-248
- [15] Kováčová, M., Takáčsová, M., Longauerová, Z: Porovnanie antioxidantných účinkov rutínu a flavonoidov pohánky. Comparison of antioxidative effects of rutine and flavonoids in buckwheat (in Slovak). In.: Proceedings of the XIII th International Conference LABORALIM 2001, B. Bystrica, Slovak Republic, February 7.-8. 2001, p. 149-151
- [16] Németh, K., Takáčsová, M., Stahelová, A.,Ambrušová, D.: Antioxidálny účinok ovsa a prosa v repkovom oleji. Antioxidative effect of oat and millet in rape seed oil (in Slovak). In: Proceedings of the XIII th International Conference LABORALIM 2001, B. Bystrica, Slovak Republic, February 7.-8. 2001, p. 189-192
- [17] Stahelová, A., Takáčsová, M., Németh, K.: Zloženie a antioxidantné vlastnosti olív a olivového oleja. Composition and antioxidative properties of olive and of olive oil (in Slovak). In: Proceedings of the XIII th International Conference LABORALIM 2001, B. Bystrica, Slovak Republic, February 7.-8. 2001, p. 218-221
- [18] Takáčsová, M., Kováčová, M., Papalová, Z.: Vplyv rozmarínu na stabilitu lipidov mäsa. Effect of rosemary on the stability of meat lipids (in Slovak). In: Proceedings of the XIII th International Conference LABORALIM 2001, B. Bystrica, Slovak Republic, February 7.-8. 2001, p. 253-255
- [19] Dodok L., Buchtová V. Hozová B. Burisová A.: Vplyv zlepšujúcich prípravkov na reologické vlastnosti cesta a finálneho

- výrobku. Influence of improvers on rheological properties of the dough and of final product (in Slovak). In: Proceedings of the XIII th International Conference LABORALIM 2001, B. Bystrica, Slovak Republic, February 7.-8. 2001, p.91-94
- [20] Burisová A., Dodok L., Ebringerová A., Hromádková Z.: Vplyv prídavku glukurónoxylánu na vlastnosti pšeničného cesta. Effect of glucuronoxylane addition on the properties of wheat dough (in Slovak). In: Proceedings of the XIII th International Conference LABORALIM 2001, B. Bystrica, Slovak Republic, February 7.-8. 2001, p. 82-86
- [21] Hromádková Z., Tomášková B., Ebringerová A., Burisová A.: Frakcionácia zložiek pohánky obyčajnej. Fractionation of buckwheat components (in Slovak). In: Proceedings of the XIII th International Conference LABORALIM 2001, B. Bystrica, Slovak Republic, February 7.-8. 2001, p. 107-113
- [22] Hybenová E., Karovičová J., Greif G., Rybárová Z.: Produkcia organických kyselín v zeleninovej šťave. Organic acids production in vegetable juices (in Slovak). In: Proceedings of the XIII th International Conference LABORALIM 2001, B. Bystrica, Slovak Republic, February 7.-8. 2001, p. 117-122
- [23] Hybenová E., Karovičová J., Greif G., Trúchla L.: Redukcia cudzorodých látok v priebehu mliečnej fermentácie. Reduction of foreign substances during lactic fermentation (in Slovak). In: Proceedings of the XIII th International Conference LABORALIM 2001, B. Bystrica, Slovak Republic, February 7.-8. 2001, p. 128-133
- [24] Karovičová J., Greif G., Hybenová E., Kohajdová Z.: Použitie PCA pri hodnotení chuti mliečne fermentovaných zeleninových štiav. Application of PCA in evaluation of taste of lactic fermented vegetable juices (in Slovak). In: Proceedings of the XIII th International Conference LABORALIM 2001, B. Bystrica, Slovak Republic, February 7.-8. 2001, p. 134-137
- [25] Karovičová J., Polonský J., Kohajdová Z., Greif G.: Validácia kapilárnej izotachofórey pri stanovení organických kyselín. Validity of capillary isotachopheresis in determination of organic acids (in Slovak). In: Proceedings of the XIII th International Conference LABORALIM 2001, B. Bystrica, Slovak Republic, February 7.-8. 2001, p. 138-143
- [26] Kohajdová Z., Karovičová J., Greif G.: Metódy stanovenia biogénnych amínov v potravinách. Methods of biogenic amine determination in foods (in Slovak). In: Proceedings of the XIII th International Conference LABORALIM 2001, B. Bystrica, Slovak Republic, February 7.-8. 2001, p. 144-148
- [27] Greif G., Greifová M., Karovičová J.: Vplyv teploty na rast vybraných fekálnych baktérií a produkciu amínov. Influence of temperature on the growth of selected fecal bacteria and on the production of amines (in Slovak). In: Proceedings of the XIII th International Conference LABORALIM 2001, B. Bystrica, Slovak Republic, February 7.-8. 2001, p. 305-310
- [28] DODOK, L., BUCHTOVÁ, V., HOZOVÁ, B., BURISOVÁ, A.: Vplyv zlepšujúcich prípravkov na tvorbu a reologické vlastnosti cesta a finálneho výrobku. Effect of improvers on the formation and on rheological properties of the dough and of final product (in Slovak). In: Proceedings of the XIII th International Conference LABORALIM 2001, B. Bystrica, Slovak Republic, February 7.-8. 2001, p. 91-94
- [29] Lenkeyová, I. Greifová, M. Staňková, A., Sádecká, Ž., Greif, G.: Vplyv konzervačných látok na rast *Enterobacter aerogenes* a produkciu biogénnych amínov. Effect of preservatives on the growth of *Enterobacter aerogenes* and on the production of biogenic amines (in Slovak). In: Proceedings of the XIII th International Conference LABORALIM 2001, B. Bystrica, Slovak Republic, February 7.-8. 2001, p. 295-304
- [30] Takáčsová, M., Kováčová, M., Nguyen, D.V.: Antioxidačný účinok extraktov cesnaku. Antioxidative effect of garlic extracts (in Slovak). In: Proceedings of XXVIII th Seminary about Food Quality, Brno 2001, Czech Republic, p. 5

### C. Books and Textbooks

- [1] Pokorný, J., Trojáková, M., Takáčsová, M.: The use of natural antioxidants in foodproducts of plant origin. In: Antioxidants in Food . Edited by Jan Pokorný, Nedyalka Yanishlieva and Michael Gordon, CRC Press Boca Raton Boston, New York, Washington DC, p. 355-372 (2001)

## CENTRAL LABORATORIES

**Head of the Department:**  
Assoc.Prof. Ján Leško, PhD

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### I. STAFF

**Associate Professors:**

Ján Leško, PhD; Ján Lokaj, PhD;

**Research Fellows:**

Štefan Holotík, PhD; Tibor Jakubík, PhD; Tibor Liptaj, PhD;

**PhD Student:**

Svatava Kašparová; Pham Tran Nghia;

**Technical Staff:**

Svatava Kašparová; Peter Kottaš; Mária Mravcová; Eva Pappová; Nad'a Prónayová; Walter Weis

### II. TEACHING AND RESEARCH LABORATORIES

#### B. Research Laboratory

Laboratory of NMR Spectroscopy (NMR)

Laboratory of Mass Spectrometry (MS)

Laboratory of X-Ray Microanalysis

### IV. CURRENT RESEARCH PROJECTS

#### A. Development of NMR techniques for the structure determination of modular molecules (Tibor Liptaj)

The main goals of the project are:

a/ development of the NMR techniques which provide long-range structural information on the studied molecules. These methods rely on measurement and interpretation of residual dipolar coupling constants which appear in high resolution spectra because of partial orientation of molecules.

The main results are:

a/ development of the methods for the precise determination of the value of coupling constants

b/ determination of the dipolar  $^1\text{J}(\text{C}-\text{H})$  coupling constants in the model oligosaccharide.

Direct participation on other projects:

NMR laboratory cooperates mainly with:

Department of organic chemistry  
Department of organic technology  
Department of petroleum technology and petrochemistry  
Department of physical chemistry  
Department of anorganic chemistry  
Department of analytical chemistry  
Department of biochemical technology  
Department of biochemistry and microbiology  
Department of plastics and rubber

MS Laboratory cooperates mainly with:

Department of organic chemistry  
Department of organic technology  
Department of petroleum technology and petrochemistry  
Department of analytical chemistry  
Department of biochemistry and microbiology

Laboratory of Microanalysis cooperates with:

Department of organic chemistry  
Department of ceramics, glass and cement

### V. COOPERATION

#### A. Cooperation in Slovakia

Faculty of Medicine, Jesenius University, Martin

Institute of Preventive and Clinical Medicine, Bratislava

Pharmacobiochemical Laboratory, Medical Faculty, Comenius University, Bratislava



Derer Hospital, Bratislava  
 Drug Research Institute, Modra  
 Slovak Academy of Sciences, Institute of Inorganic Chemistry, Bratislava  
 Slovak Academy of Sciences, Chemical Institute, Bratislava  
 Viticultural and Enological Research Institute, Šenkvice  
 Comenius University, Faculty of Natural Sciences, Bratislava  
 Comenius University, Faculty of Pharmacy, Bratislava  
 Science and Conservation Research Institute Bratislava  
 Research Institute of Animal Production, Nitra  
 Chemical Factory, Nováky  
 Slovnaft, Bratislava  
 Duslo, Šaľa  
 Slovakofarma, Hlohovec  
 Glass Factory, Nemšová  
 Ceramics Factory, Čáb  
 Technical Glass Factory, Bratislava

## B. International Cooperation:

The University of Edinburgh, Chemistry Department, The King's Buildings, Edinburgh, England  
 - Development of NMR techniques for structure determination of multi-modular proteins  
 Université Blaise Pascal, Department of Organic and Bioorganic Chemistry, Clermont-Ferrand, France  
 - The NMR study of the cellular metabolism of the *Fibrobacter succinogenes* using C-13 labelled substrate  
 Università di Bari, Facoltà di Medicina Veterinaria, Istituto di Clinica Chirurgica, Italy  
 - Study of the ischemia and reperfusion on the metabolic map of rabbit CNS.  
 Department of Fine Organic Chemistry, ECPM/ University L. Pasteur, Strasbourg, France  
 - NMR characterization of chiral compounds

## C. Membership in Domestic Organizations and Society:

Slovak Spectroscopic Society, Bratislava (T.Liptaj)

## G. Visitors from Abroad:

Prof. Dušan Uhrín The University of Edinburgh, England, March 2001 (11 days)  
December 2001 (11 days)

## H. Visits of Staff Members and PhD Students to Foreign Institutions:

Pham Tran-Nghia The University of Edinburgh, England, January - February 2001, (14 days)  
Tibor Liptaj Université Blaise Pascal, Department of Organic and Bioorganic Chemistry, Clermont-Ferrand, France, January – April 2001 (95 days)

# VII. PUBLICATIONS

## A. Journals (\*registered in Current Contents)

- [1]\* Blanáriková I., Dugovič B., Fišera L., Hametner C., Prónayová N.: 1,3-Dipolar cycloadditions of D-erythrose- and D-threose-derived nitrones to maleimides. *Arkivoc* 2(2), 1091-1103 (2001)
- [2]\* Bobošíková M., Clegg W., Coles S.J., Dandárová M., Hursthouse M.B., Kiss T., Krutošíková A., Liptaj T., Prónayová N., Ramsden C.A.: The oxidative rearrangement of furan-2-carboximidamides: preparation and properties of 2-acylamino-furans. *J. Chem. Soc., Perkin Trans. 1* (7), 680-689 (2001)
- [3]\* Čákr M., Hercegová A., Leško J., Polonský J., Sádecká J., Skačáni I.: Isotachophoretic determination of naproxen in the presence of its metabolite in human serum. *J. Chromatogr. A*, 916, 207-214 (2001)
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