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Fields of research

- Hydrodynamics of two phase flow in micro channels
- Sulfur dioxide oxidation, sulfation and sulfonation
- Kinetic studies of heterogeneously catalyzed reactions in microreactor
- Design of counter-current vibrating plate extractor (VPE)
- Fluorinated hydrocarbons as potential solvents in liquid-liquid extraction processes
- Supercritical fluid extraction of biologically active substances
- Chemical and enzymatic reactions in supercritical CO_2
- Mass transport through ionic liquid membranes
- Membrane separation of methane and CO_2
- Separation of racemic mixtures
- Separation of gasoline vapors from air by supported ionic liquids membranes
- Condensation in porous membranes during vapor permeation

Applied research

- Hydrodynamic characterization of micromixers
- Heat and mass transfer of liquid flow in microreactors
- Liquid-liquid extraction of luminophores, recycling of Y and Eu
- Liquid-liquid and supercritical fluid extraction and refining of plant extracts
- Purification of biogas by supported liquid membrane

Research projects

Flexible, fast and future production processes (F^3 Factory)

(V. Jiřičný, jiricny@icpf.cas.cz; FP7 collaborative large integrated project, Theme NMP-2008-3.2-1; supported by EU under Contract No. CP-IP 228867-2 F^3 Factory)

The goals of the projects are in improvements of EU chemical industry's competitive position by development modular continuous plant (F^3 Plant) which combines world scale continuous plant efficiency, consistency and scalability with the versatility of batch operation. Based on the extensive hydrodynamic study, the microsulphonator pilot plant prototype was designed, manufactured and tested in ICPF. Together with Procter&Gamble, ICPF participated in the upgrade of the industrial pilot plant with the aim of installing the new microsulphonator reactor. The installation of microsulphonator into Procter&Gamble pilot plant is foreseen for early 2013. ICPF team also defined an advanced method for the SO_2 analysis suitable for the pilot plant installation. We also participated in the design of pilot plant size microreactor for sulfur dioxide catalytic heterogeneous oxidation.

Gas-liquid electrochemical microreactors - role of hydrodynamics

(J. Křišťál, kristal@icpf.cas.cz; bilateral project ASCR-CNRS, project No. 22540)

The proposed project deals with the study of hydrodynamics of the gas-liquid flow generated by an electrochemical reaction in a low aspect ratio microreactor. Objective is to better understand and characterize the effect of gas flow and bubbles on the performance of liquid electrochemical reactions being performed in the electrochemical microreactor. [Ref. 14]

Schematic diagram of the T-junction microchannel (left) and the topology of the curved (center) and right-angled (right) meandering microchannels

Refining of biologically active therapeutic substances from coniferous wood

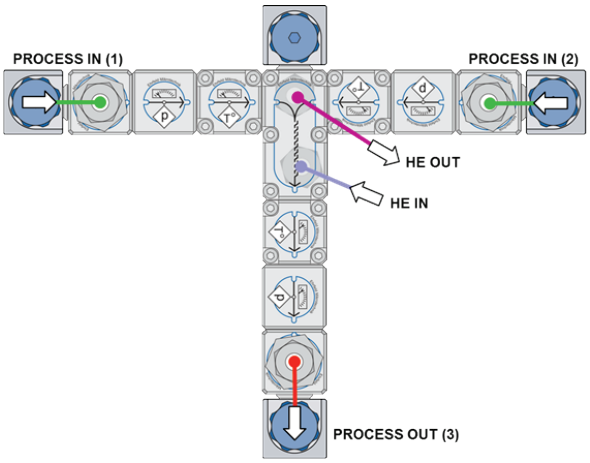
(A. Heyberger, heyberger@icpf.cas.cz; contract with Favea Europe Ltd.)

The object of this contract was to perform laboratory and pilot plant tests for refining of liquid coniferous extracts using countercurrent vibrating plate extractor (VPE). The experimental results were used as a basis for the design of the operating extractor to replace the existing batch production.

Research and developments of various microapparatus characteristics

(J. Křišťál, kristal@icpf.cas.cz; contract with Procter&Gamble)

The contract deals with experimental measurement of various microapparatuses (preferably mixers) and determination of their hydrodynamic characteristics with respect to various physical-chemical properties selected liquids. The collected data and developed methodology of micromixer selection will form databasis for design and development of new chemical processes. Results published in three confidential Procter&Gamble research reports.



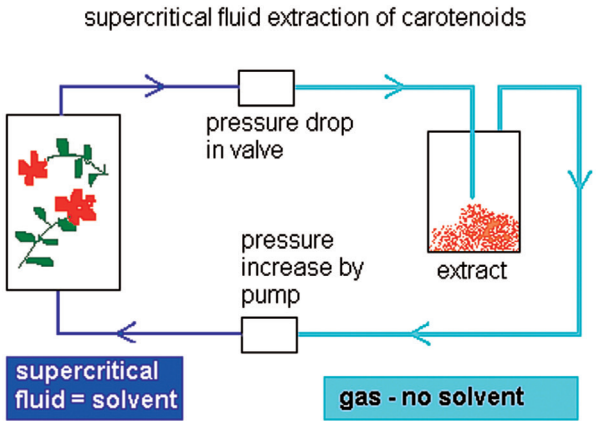
Visualization of the experimental set-up for testing of micro mixers

Research and development of new products for complex plant protection

(M. Sajfrtová, sajfrtova@icpf.cas.cz; joint project with Matoušek CZ a.s., Crop Research Institute; supported by TACR, project No. TA01010578)

New preparations for eco-agriculture are being developed on the basis of hydrodistillates and supercritical extracts from tropical plants with high content of the biologically active substances.

Plant material supplied from South Africa is submitted to supercritical fluid extraction, hydrodistillation and maceration in order to assess the suitability of the methods used for obtaining extracts with maximum biological activity. The supercritical fluid extraction is conducted under different experimental conditions. The insecticidal activity (antifeedancy, acute toxicity, and chronic toxicity) of isolates is measured on larvae of *Spodoptera litoralis*. Antifungal bioassay is carried out on the isolates as the inhibition effect on the growth of model pathogenic and toxinogenic fungi. The chemical composition of isolates is determined by GC/MS technique. [Refs. 2, 9-12]



Study of polymeric membrane swelling and make use of this effect for increasing its permeability

(P. Uchytil, uchytil@icpf.cas.cz; joint project with IMC, supported by the GACR, project No. P104/09/1165)

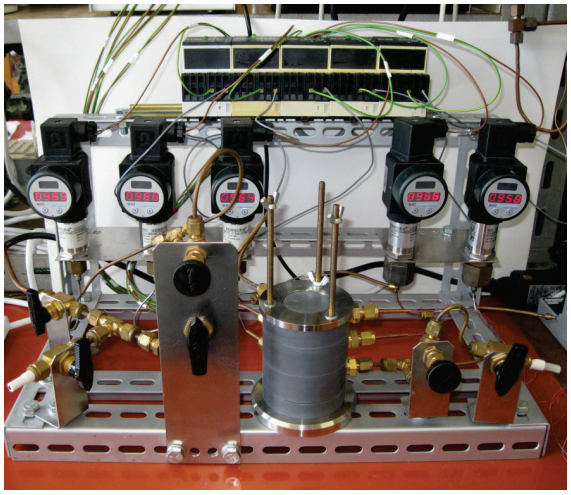
The location of the phase change inside membranes and swelling of the membrane material during toluene transport in a polyethylene membrane were investigated. The special

experimental sweeping-gas set-up was proposed and constructed to obtain all transport parameters in polymeric membranes (flux, diffusivity and sorption). Study of an addition of a convenient substance was performed on several types of membranes that were prepared in cooperation with the foreign partner (Prof. S.-Y. Suen). On the basis of the obtained results new membrane separation process was designed and the high separation efficiency of gas separation was experimentally verified and applied for patent. [Ref. 15]

Flow of saturated vapors through porous membranes

(J. Řezníčková, reznickova@icpf.cas.cz; joint project with Institut für Strömungsmechanik und Wärmeübertragung Technische Universität Wien; supported by MEYS, MOBILITY, project No. 7AMB12AT010)

Aim of our collaboration is to carry out a series of experiments to obtain the pressure and temperature distributions within asymmetric ceramic membranes. Experimental data improve our understanding of the permeation process especially under condition of condensation. It is difficult to set and maintain the correct experimental conditions. Furthermore, the direct measurement of the temperature and pressure distributions is not possible. Experimental difficulties are one of the reasons for the lack of sufficient experimental data. Therefore, a special apparatus was designed and constructed. The use of this apparatus helped at obtaining at least in an indirect way the desired pressure and temperature distributions. The data gleaned from our experiments help at understanding the flow process. By condensation it may be possible to enhance the production in similar processes.

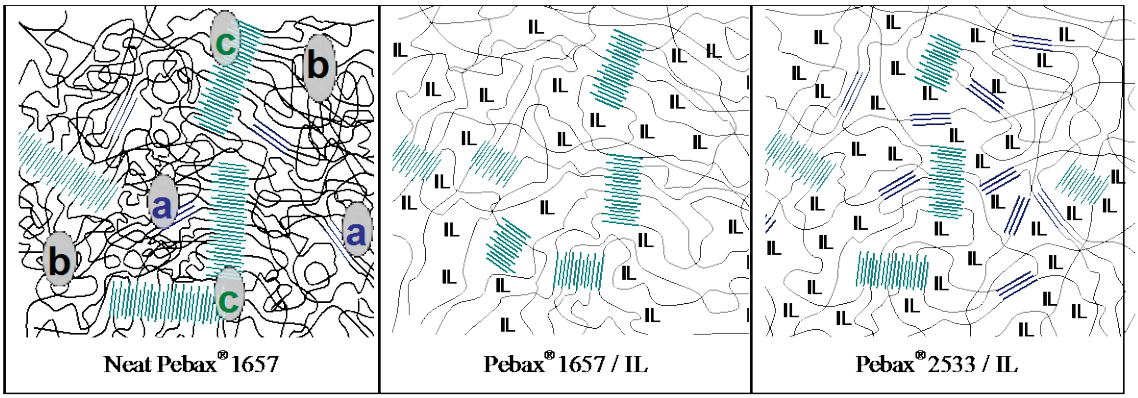


Apparatus for vapor permeation transport connected with condensation

Separation of volatile organic compounds (VOCs) from air

(P. Izák, izak@icpf.cas.cz; joint project with ICT Prague; supported by GACR, project No. P106/10/1194)

Aim of this project is a development and application of membrane techniques to increase the affectivity of classical separation processes with help of computer simulations and theoretical modeling. In most of processes the goal of separation techniques is to recycle vapor phase, which was lost in a sweeping gas. Optimization of polymeric membrane for specific separation task is time consuming and financial demanding. Ionic liquids have a great potential for membrane processes especially if only a small amount of ionic liquid is necessary e.g. supported ionic liquid membranes (SILMs). Characteristic property of ionic liquid is their very low vapor pressure, which makes them attractive for gas and vapor permeation. [Refs. 1, 4, 5, 6, 8]



Schematic representation of the microstructure of pure Pebax® (left), Pebax®1657/IL gel (middle), and Pebax®2533/IL gel (right). Domain identification: a = crystalline PE blocks; b = amorphous soft PE blocks and amorphous hard PA blocks, c = crystalline hard PA blocks, IL = dissolved [BMIM][OTf]

Membrane separation - the more effective separation of a pure enantiomer from a racemic mixture

(P. Izák, izak@icpf.cas.cz; joint project with ICT Prague and IMC; supported by GACR, project No. P106/12/0569)

Drug stereochemistry has become an issue for the pharmaceutical industry and the regulatory authorities, because each of the enantiomers frequently shows different impacts to living organisms. The goal of the proposal is to develop new membrane separation techniques for successful resolution of racemic mixtures allowing optimization of the therapeutic value of enantiomeric drugs (pharmacological and toxicological) and avoiding their adverse effects. The key objective is to separate enantiomers by a new membrane separation method, based on the proposed supported chiral room temperature ionic liquid membrane, that has never been studied yet. In comparison with classical methods employed earlier, it should show higher efficiency and cost effectiveness in the processes of enantiomer separation. To greatly reduce the amount of experimental work, particle-based modeling will be employed. After gathering all transport characteristics, it will be possible to model the separation process and to estimate permeability and selectivity of the separation.

International co-operations

CNRS Toulouse, France: Two phase flow hydrodynamics in microchannels

CSIR of Pretoria and Johannesburg, Republic of South Africa: Extraction of essential oils from plant raw materials

Institut für Strömungsmechanik und Wärmeübertragung Technische Universität Wien: Flow of saturated vapors through porous membranes

Institute of Chemical Engineering, Sofia, BAS: High-pressure phase equilibria

Institute of Macromolecules, St. Petersburg, RAS, Russia: Membrane separation

Institute on Membrane Technology, CNR, Italy: Novel composite membranes containing ionic liquid and selected polymers for specific gas/gas, gas/vapor and vapor/vapor separations

KIT Karlsruhe, Germany: Design of pilot plant size microreactor for sulfur dioxide catalytic heterogeneous oxidation

National Chung Hsing University, Taiwan: Preparation of Dense Homogeneous Polymeric Membranes and Study on Their Gas Permeation Properties

Otto von Guericke University of Magdeburg, Germany: Mass transport through porous membranes
Procter&Gamble, Belgium: Research and developments of microapparatus characteristics
Procter&Gamble: Hydrodynamics of micro reactor for sulfonation
Technische Universität Wien, Institut für Strömungslehre und Wärmeübertragung, Austria: Flow of saturated vapors through porous membranes
Technical University of Lisbon, Portugal: Supercritical extraction of biological compounds from aromatic plants
University of Colorado, Boulder, CO, USA: Mass transport during vapor permeation and pervaporation, ionic liquids
University of Burgos, Spain: Enzymatic reactions of oil in supercritical CO_2 medium
University of KwaZulu-Natal, Republic of South Africa: Liquid-liquid extraction processes with fluorinated hydrocarbons, recovery of luminophores

Visits abroad

J. Křišťál, CNRS, Toulouse, France (1 week)
P. Uchytil, National Chung Hsing University, Taichung, Taiwan (3 weeks)
A. Heyberger, University of KwaZulu-Natal, Durban, Republic of South Africa (3 weeks)

Visitors

J. Aubin, CNRS Toulouse, France
A. Bucić-Kojić, Faculty of Food Technology, Osijek University, Croatia
M. Čársky, University of KwaZulu-Natal, Durban, Republic of South Africa
J. Heck, C. Raffa, Ehrfeld Mikrotechnik BTS, Germany
A. Palavra, Technical University of Lisbon, Portugal
A. Martin, ENSIASET, Toulouse, France
A. Simmoncelli, Procter&Gamble, Belgium
R.P. Stateva, Inst. Chem. Eng. BAN, Sofia, Bulgaria

Teaching

P. Izák: ICT, Faculty of Chemical Engineering, postgraduate course “Physical chemistry for technological practice”
J. Hanika: ICT, Faculty of Chemical Technology, postgradual course “Multiphase reactors”
J. Hanika: ICT, Faculty of Chemical Technology, course “Pharmaceutical engineering”
H. Sovová: ICT, Faculty of Chemical Engineering, postgraduate course “Properties and application of supercritical fluids”

Publications

Original papers

[1] Bernardo P., Jansen J.C., Bazzarelli F., Fuoco A., Friess K., Izák P., Jarmarová V., Kačírková M., Clarizia G.: Gas Transport Properties of PEBAX®/Room Temperature Ionic Liquid Gel Membranes. *Sep. Purif. Technol.* 97(SI), 73-82 (2012).

[2] Coelho J.P., Cristino A.F., Mantos P.G., Rauter A.P., Nobre B.P., Mendes R.L., Barroso J.G., Mainar A., Urieta J.S., Fareleira J.M.N.A., Sovová H., Palavra A.F.: Extraction of Volatile Oil from Aromatic Plants with Supercritical Carbon Dioxide: Experiments and Modeling. *Molecules* 17(9), 10550-10573 (2012).

[3] Drhová M., Hejda S., Křišťál J., Klusoň P.: Performance of Continuous Micro Photo Reactor – Comparison with Batch Process. *Procedia Eng.* 42(SI), 1365-1372 (2012).

[4] Friess K., Jansen J.C., Bazzarelli F., Izák P., Jarmarová V., Kačírková M., Schauer J., Clarizia G., Bernardo P.: High Ionic Liquid Content Polymeric Gel Membranes: Correlation of Membrane Structure with Gas and Vapour Transport Properties. *J. Membr. Sci* 415, 801-809 (2012).

[5] Izák P., Kárászová M., Vejražka J., Friess K., Randová A., Jansen J.C.: The Effective Upgrading of Raw Biogas to Methane by Selective Membranes. *Procedia Eng.* 44, 429-431 (2012).

[6] Kárászová M., Vejražka J., Veselý V., Friess K., Randová A., Hejtmánek V., Brabec L., Izák P.: A Water-Swollen Thin Film Composite Membrane for Effective Upgrading of Raw Biogass by Methane. *Sep. Purif. Technol.* 89, 212-216 (2012).

[7] Křišťál J., Kodym R., Bouzek K., Jiřičný V., Hanika J.: Electrochemical Microreactor Design for Alkoxylation Reactions – Experiments and Simulations. *Ind. Eng. Chem. Res.* 51(4), 1515-1524 (2012).

[8] Lísal M., Posel Z., Izák P.: Air-Liquid Interface of Imidazolium-Based [Tf_2N-] Ionic Liquids: Insight from Molecular Dynamics Simulations. *Phys. Chem. Chem. Phys.* 14, 5164-5177 (2012).

[9] Sajfrtová M., Sovová H.: Solute-matrix and Solute-Solute Interactions during Supercritical Fluid Extraction of Sea Buckthorn Leaves. *Procedia Eng.* 42(SI), 1682-1691 (2012).

[10] Sovová H.: Modeling the Supercritical Fluid Extraction of Essential Oils from Plant Materials. *J. Chromatogr., A* 1250(SI), 27-33 (2012).

[11] Sovová H.: Steps of Supercritical Fluid Extraction of Natural Products and Their Characteristic Times. *J. Supercrit. Fluids* 66(SI), 73-79 (2012).

[12] Sovová H.: Apparent Solubility of Natural Products Extracted with Near-Critical Carbon Dioxide. *Am. J. Anal. Chem.* 3(12A), 958-965 (2012).

[13] Vajglová Z., Veselý M., Křišťál J., Vychodilová H., Tříska J., Jiřičný V.: Photochemical Degradation of Polybrominated Diphenyl Ethers in Micro Photo-Reactor. *Procedia Eng.* 42(SI), 1378-1382 (2012).

[14] Záloha P., Křišťál J., Jiřičný V., Völkel N., Xuereb C., Aubin J.: Characterisation of Liquid Slugs in Gas-Liquid Taylor Flow in Microchannels. *Chem. Eng. Sci.* 68(1), 640-649 (2012).

[15] C.-Y. Liang, P. Uchytil, R. Petrychkovych, Y.-C. Lai, K. Friess, M. Sipek, M. M. Reddy, S.-Y. Suen, Preparation of PES (polyethersulfone)/MMT (Na-montmorillonite) and PES/TiO2 mixed matrix membranes for CO2/CH4 separation, Sep. Purif. Technol. 92, 57-63 (2012).

Chapters in books

[16] Hanika J.: Chemie na konci světa. (Czech) Chemistry in Ending World. In: Tři svíce za budoucnost. (Cílek, V., Ed.), pp. 44-54, Novela bohemica, Praha 2012.

[17] Kárászová M., Friess K., Šípek M., Jansen J.C., Izák P.: Chapter 3: Biogas Upgrading for the 21st Century. (Litonjua, R.; Cvetkovski, I., Ed.), Nova Science Publishers, New York 2012.

[18] Izák P., Kárászová M.: Pervaporace. (Czech) Pervaporation. In: Membránové procesy. (Palatý, M., Ed.), VŠCHT, Praha 2012.

Patents

[19] Izák P., Kárászová M., Vejražka J.: Způsob separace plynné směsi a zařízení k provádění tohoto způsobu. (Czech) A Process for the Separation of a Gaseous Mixture and an Apparatus for Carrying Out the Same. Pat. No. CZ303107/PV 2010-438. Applied: 11.06.20, patented: 12.04.04.

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[21] Lederer J., Kovač D., Veselý V., Hanika J., Nečesaný F.: Způsob výroby vodíku parciální oxidací vysokovroucích uhlovodíkových směsí a biomasy, a zařízení k provádění způsobu. (Czech) Process for Hydrogen Production by Partial Oxidation of High Boiling Hydrocarbon Mixtures and Biomass, and Apparatus for Processing. Pat. No. CZ303392/PV 2010-653. Applied: 10.09.02, patented: 12.08.29.