Molecular Modelling and Simulation for Industrial Applications: Physico-Chemical Properties and Processes

EFCE Working Party on Thermodynamics and Transport Properties

ProcessNet Working Party "Molecular Modelling and Simulation for Process and Product Design"

March 22 - 23, 2010 in Würzburg / Germany

Programme and Call for Posters

EFCE-Event No. 687

www.processnet.org/mol_eng_methods

organised in cooperation with

Priority Programme 1155 "Molecular Modelling and Simulation in Process Engineering" of Deutsche Forschungsgemeinschaft.

Monday, March 22, 2010

11:00 **Opening:**
I.G Economou, The Petroleum Institute, Abu Dhabi/UAE and National Center for Scientific Research "Demokritos" Athens/GR;
H. Hasse, TU Kaiserslautern/D

Plenary Lectures I

11:10 **Adsorptive separations of fluid mixtures using nano-porous materials: how can molecular simulations help in designing the right adsorbent?**
A. Fuchs, Chimie ParisTech, Paris/F

11:45 **Structure, solvation, and phase equilibria in multicomponent systems**
I. Siepmann, University of Minnesota, Minneapolis, MN/USA

12:20 **Applied thermodynamics in industry – a pragmatic approach**
E.M. Hendriks, Shell Global Solutions International B.V., Amsterdam/NL

12:55 **Lunch Break**

Session I: Molecular Simulation of Physico-Chemical Properties

14:05 **Thermophysical properties from anisotropic united atoms potentials: a review**
P. Ungerer, N. Ferrando, V. Lachet, C. Nieto-Draghi, B. Creton, IFP, Rueil-Malmaison/F;
J. Perez-Pellitero, IFP, Lyon/F; P. Malfreyt, F. Biscay, Université Blaise Pascal, Clermont-Ferrand/F;
A. Mackie, ETSEQ-URV, Tarragona/E; B. Rousseau, CNRS-Université Paris 11, Orsay/F; A. Boutin, ENS, UPMC-CNRS, Paris/F; E. Bourasseau, CEA-DAM, Bruyères le Chatel/F

14:35 **Molecular simulation of diffusion and solubility of hydrogen, carbon monoxide and water in heavy n-alkanes**
Z. Makrodimitri, I.G. Economou, The Petroleum Institute, Abu Dhabi/UAE and National Center for Scientific Research "Demokritos", Athens/GR; D.J.M. Unruh, Shell Global Solutions International B.V., Amsterdam/NL

14:55 **Computing the solubility of CO_2, CH_4, N_2 and O_2 in Imidazolium-based ionic liquids**
D. Kerlé, Universität Rostock/D; D. Paschek, Rensselaer Polytechnic Institute, Troy, NY/USA; R. Ludwig, Universität Rostock/D

15:15 **Thermal expansion of water near surface**
A. Oleinikova, I. Brovchenko, TU Dortmund/D

15:35 **Molecular dynamics calculations of solid-liquid interfacial tensions and contact angles**
F. Leroy, F. Müller-Plathe, TU Darmstadt/D

15:55 **Coffee Break**

	Session II: Nanoscale Processes	Session III: Advanced Engineering Methods A
16:20	**Molecular dynamics simulation of particle formation by rapid expansion of a supercritical solution (RESS)** F. Römer, T. Kraska, University of Cologne/D	**Intramolecular association within the SAFT framework** A. Avlund, G.M. Kontogeorgis, M.L. Michelsen, Technical University of Denmark, Kgs. Lyngby/DK; W.G. Chapman, Rice University, Houston, TX/USA
16:40	**Steady-state molecular dynamics simulation of nucleation and droplet surface properties in a supersaturated vapor** J. Vrabec, M. Horsch, S. Miroshnichenko, University of Paderborn/D; M. Bernreuther, HLRS, Stuttgart/D; H. Hasse, TU Kaiserslautern/D	**Use of experimental association energies to guide the parametrization of cross-association phenomena using the polar PC-SAFT with group contributions (GC-PPC-SAFT) equation of state: application to vapour-liquid and liquid-liquid equilibria of water** D. NguyenHuynh, J.C. de Hemptinne, R. Lugo, IFP, Rueil-Malmaison/F; J.P. Passarello, P. Tobaly, LIMHP, Villetaneuse/F
17:00	**Transport of guest molecules through a membrane containing microporous crystals and mesopores** S. Fritzsche, University of Leipzig/D; S. Vasenkov, University of Florida, Gainesville, FL/USA; M. Knauth, University of Leipzig/D	**Fluid viscosity - how molecular modelling helps** V. Vesovic, Imperial College London/UK
17:20	**Atomistic model of two commercial reverse osmosis membranes** R. Kieffer, AgroParisTech, Massy/F; O. Vitrac, AgroParisTech - INRA, Massy/F; B. Rousseau,Université de Paris Sud - CNRS UMR 8000, Orsay/F; C. Fargues, M.-L. Lameloise, AgroParisTech, Massy/F	**Thermodynamic modeling of polyelectrolyte aqueous two-phase systems** S. Naeem, G. Sadowski, TU Dortmund/D
17:40	**Simulation of adsorption and phase transitions of gases on metal surfaces - oxygen on Ni(111) as an example** C. Lazo, F.J. Keil, TU Hamburg-Harburg/D	**Phase equilibria in systems containing large molecules: combination of MD and COSMO-RS** P. Yamin, L. Mokrushina, University of Erlangen-Nürnberg, Erlangen/D; I. Smirnova, TU Hamburg-Harburg/D; W. Arlt, University of Erlangen-Nürnberg, Erlangen/D
18:00	**Poster Session (until 20.00)**	
19:00	**Meeting EFCE Working Party (until 20:00)**	
20:30	**Conference Dinner**	

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Tuesday, March 23, 2010

Plenary Lectures II

08:15 **Modeling of electrolyte and polyelectrolyte systems**
G. Sadowski, TU Dortmund/D

08:50 **Molecular base group-contribution theories for the fluid phase equilibria and derivative properties of complex fluids: the SAFT-γ approach**
G. Jackson, Imperial College London/UK

09:25 **Molecular modeling of polymer rheology: an ultra-sensitive characterization tool**
R. Larson, University of Michigan, Ann Arbor, MI/USA

10:00 **Coffee Break**

	Session IV: MD/MC Simulation Methods and Tools	Session V: Advanced Engineering Methods B
10:25	**Sampling methods for molecular simulations of the adsorption from dilute solutions** S. Leroch, M. Wendland, J. Fischer, University of Natural Resources and Applied Life Sciences, Vienna/A	**A force field for fluoropropenes, including HFO-1234yf** G. Raabe, TU Braunschweig/D; E.J. Maginn, University of Notre Dame, IN/USA
10:45	**On the estimation of partition coefficients from molecular dynamics simulations** N. Garrido, M. Jorge, A.J. Queimada, University of Porto/P; I.G. Economou, The Petroleum Institute, Abu Dhabi/UAE and National Center for Scientific Research "Demokritos" Athens/GR; E.A. Macedo, University of Porto/P	**Using non-cubic simulation boxes in isobaric Monte Carlo simulations of solids and dense fluids** B. Wittich, U.K. Deiters, University of Cologne/D
11:05	**Multi-particle sampling methods in Monte Carlo simulations on fluids** I. Nezbeda, F. Moucka, Academy of Science, Prague/CZ	**Unit operations simulated on the molecular level** A. Pereira Neto, D. Babic, A. Pfennig, RWTH Aachen/D
11:25	**Molecular-level dew-point simulation methodology for multi-component mixtures and application to refrigerant cycle design** M. Francova, Jan Evangelista Purkinje University, Ústí nad Labem/CZ; M. Kowalski, W.R. Smith, University of Ontario, Oshawa/CDN; I. Nezbeda, Academy of Sciences of the Czech Republic, Prague/CZ	**Calculation of thermophysical properties of hydrogen sulfide in the gas phase based on an ab initio intermolecular potential energy surface** R. Hellmann, E. Bich, E. Vogel, University of Rostock/D; A.S. Dickinson, Newcastle University, Newcastle upon Tyne/UK; V. Vesovic, Imperial College London/UK
11:45	**ms2: a molecular simulation tool for thermo-dynamic properties** J. Vrabec, University of Paderborn/D; S. Deublein, G. Guevara, T. Merker, H. Hasse, TU Kaiserslautern/D; M. Bernreuther, HLRS, Stuttgart/D	**Treatment of multipole-shape couplings in predictive equation of state models** K. Leonhard, RWTH Aachen/D

12:05 **Lunch Break**

Session VI: Industrial Applications of Molecular Simulation

13:05 **Molecular simulation methods in industrial research and development**
J. Vorholz, Evonik Industries, Darmstadt/D; R. Franke, Evonik Industries, Marl/D

13:25 **Forward/backward mapping of molecular simulation and thermodynamic equations of state**
F. Heilmann, BASF SE, Ludwigshafen/D

13:45 **Molecular modelling and simulation of vapor-liquid equilibria of toxic fluids for process engineering applications**
Y. Huang, J. Vrabec, University of Paderborn/D; M. Heilig, BASF SE, Ludwigshafen/D; H. Hasse, TU Kaiserslautern/D

14:05 **Automating van der Waals parameter development**
S. Robertson, J.J. Liang, R. Akkermans, S. Todd, G Fitzgerald and G. Goldbeck, Accelrys Limited, Cambridge/UK

14:25 **Coffee Break**

Session VII: Molecular Simulation of Polymers

14:50 **Modelling of hydrogel swelling**
K. Poschlad, S. Enders, TU Berlin/D

15:10 **Molecular simulation study of the volume transition of hydrogels**
J. Walter, TU Kaiserslautern/D; J. Vrabec, University of Paderborn/D; H. Hasse, TU Kaiserslautern/D

15:30 **Modelling and design of unfolded proteins for improved superabsorbents**
T. Gebäck, P. Ahlström, University of Borås/S

15:50 **Tracer- and self-diffusion of oligomers in entangled and non-entangled polymer matrices**
M. Durand, CNRS, Institut Charles Sadron, Strasbourg/F; O. Vitrac, INRA, JRU 1145, Massy/F; H. Meyer, CNRS, Institut Charles Sadron, Strasbourg/F

16:10 **Study of the properties of imprinted PVA/PAA hydrogels by computational analysis**
M. Stannek, H.-J. Bart, TU Kaiserslautern/D

16:30 **Closing remarks**

16:45 **Geschäftssitzung des Fachausschusses Molecular Modelling (nur berufene Mitglieder)**

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Poster Programme

Advanced engineering methods

P 01 **A generalized Flory-Huggins approach of the partitioning of bulky solutes between polymers and interacting liquids**
O. Vitrac, G. Gillet, INRA, JRU 1145, Massy/F

P 02 **Modelling of phase equilibria with CPA using the homomorph approach**
M.P Breil, I. Tsivintzelis, G.M. Kontogeorgis, Technical University of Denmark, Kgs. Lyngby/DK

P 03 **High-pressure phase equilibria for carbon dioxide (1) + 1-pentanol (2) binary system**
C. Secuianu, Imperial College London/UK and Politehnica University of Bucharest/RO; V. Feroiu, D. Geana, Politehnica University of Bucharest/RO; Martin Trusler, Imperial College London/UK

P 04 **The thermodynamic consistency of binary constant-pressure VLE data determined using the two-suffix Margules equation which best satisfies the Gibbs-Duhem equation**
S. Kato, Tokyo Metropolitan University, Hachiohji/J

P 05 **Thermodynamics of carbon dioxide capture from flue gases using gas hydrate technology**
I. Ben Attouche Sfaxi, R. Lugo, IFP, Rueil Malmaison/F; A. Mohammadi, D. Richon, Ecole des Mines de Paris-Laboratoire TEP/CEP, Fontainebleau/F

P 06 **Thermodynamic modelling of hyperbranched polymers**
T. Zeiner, S. Enders, TU Berlin/D; D. Browarzik, University of Halle-Wittenberg/D

P 07 **Simple model for sigma - phase in binary alloy**
G. Rusakov, Institute of Metal Physics of the Ural Division of the Russian Academy of Sciences, Ekaterinburg/RUS; L. Son, Ural State Pedagogical University, Ekaterinburg/RUS; M. Trachtman, Institute of Metallurgy of the Ural Division of the Russian Academy of Sciences, Ekaterinburg/RUS

P 08 **Determination of the global phase behaviour of mixtures containing methane, carbon dioxide and water using the SAFT-VR approach**
J. M. Míguez, M. M. Piñeiro, Universidade de Vigo/Spain F.J. Blas, Universidad de Huelva/Spain

MD/MC Simulation Methods and Tools

P 09 **Interactions between aminoacids and inorganic salt ions in aqueous environments: molecular dynamics simulation studies**
L. Tomé, University of Aveiro/P; M. Jorge, University of Porto/P; J.R.B. Gomes, J.A.P. Coutinho, University of Aveiro/P

P 10 **What about water in modelling the morphology of crystals?**
C. Schmidt, C. Yürüdü, J. Ulrich, University of Halle-Wittenberg/D

P 11 **Prediction of alcohol + hydrocarbons phase equilibria by Monte Carlo simulation, application to an ethanoled gasoline**
N. Ferrando, V. Lachet, IFP, Rueil-Malmaison/F; A. Boutin, ENS, Paris/F

P 12 **Modelling of partition coefficients of additives in polymer/solvent systems by free energy calculations**
R. Lundsgaard, G.M. Kontogeorgis, Technical University of Denmark, Kgs. Lyngby/DK; I.G. Economou, The Petroleum Institute, Abu Dhabi/UAE and National Center for Scientific Research "Demokritos", Athens/GR

P 13 **Molecular-level simulation of electrolyte system solubility and chemical speciation**
J. Jirsak, J. Skvor, Jan Evangelista Purkyn University, Ústí nad Labem/CZ; W.R. Smith, University of Ontario, Oshawa/CDN; I. Nezbeda, Academy of Sciences of the Czech Republic, Prague/CZ

Molecular Simulation of Physico-Chemical Properties

P 14 **Prediction of transport properties of hydrogen bonding liquids by molecular simulation**
G. Guevara-Carrion, TU Kaiserslautern/D; J. Vrabec, University of Paderborn/D; H. Hasse, TU Kaiserslautern/D

P 15 **Molecular simulation of electrolyte solutions - new ion models**
S. Deublein, TU Kaiserslautern/D; J. Vrabec, University of Paderborn/D; H. Hasse, TU Kaiserslautern/D

P 16 **Thermodynamic properties for the heterogeneously catalyzed selective oxidation of cyclohexane in carbon dioxide expanded media by experiment and molecular simulation**
T. Merker, TU Kaiserslautern/D; J. Vrabec, Universität Paderborn/D; H. Hasse, TU Kaiserslautern/D

P 17 **Analysis of the structure and thermodynamic properties of methanol at 1 bar using the two-fluid theory in MC simulations**
P. Gomez Alvarez, A. Dopazo-Paz, D. Gonzales-Salgado, L. Romani, University of Vigo, Ourense/E

P 18 **Ab initio molecular dynamics simulations applied to associated liquids, mixtures and solutions**
M. Brehm, M. Kohagen, J. Thar, P. Tulip, B. Kirchner, Universität Leipzig/D

P 19 **Dynamical properties in ionic liquids via MD simulations**
A. Arnold, C. Holm, F. Dommert, Universität Stuttgart/D

P 20 **Universal description of fluid density profiles near solid surfaces**
I. Brovchenko, A. Oleinikova, TU Dortmund/D

P 21 **Augmented property prediction of ionic liquids by means of a gradient-based optimization workflow (GROW)**
T. Köddermann, M. Hülsmann, D. Reith, Fraunhofer Institut SCAI, Sankt Augustin/D

P 22 **GROW: a gradient-based optimization workflow for model building beyond manual intervention**
T. Köddermann, M. Hülsmann, D. Reith, Fraunhofer Institut SCAI, Sankt Augustin/D, J. Vrabec, Institut fuer Thermodynamik und Energietechnik, Universität Paderborn/D

Nanoscale Processes

P 23 **Investigation of gas adsorption capacity of pristine single-wall carbon nanotubes**
G. Lithoxoos, A. Lambropoulos, National Center for Scientific Research "Demokritos", Athens/GR; L. Peristeras, Scienomics, Athens/GR; N. Kanellopoulos, I.G. Economou, The Petroleum Institute, Abu Dhabi/UAE and National Center for Scientific Research "Demokritos", Athens/GR

P 24 **Separation of the Tröger's base enantiomers on the Whelk-O1 stationary phase: a molecular dynamics study**
S. Melnikov, A. Seidel-Morgenstern, Max-Planck-Institut für Dynamik komplexer technischer Systeme Magdeburg/D

P 25 **Pair interactions in transition metals at different atomic densities**
N. Dubinin, Institute of Metallurgy of the Ural Division of the Russian Academy of Sciences, Ekaterinburg/RUS

Submission of Poster Abstracts

Submission of abstracts for posters are still welcome. For detailed information please visit our conference website

www.processnet.org/mol_eng_methods

Abstracts should be submitted via file upload at the website until **February 28, 2010**.

Abstracts of maximum one page (max. 500 kb), including figures should explicitly state the objectives, new results and the conclusions or significance of the work.

Conference Office

DECHEMA e.V.

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Registration Fees [1)]

	Members [2)]	Others
from industry	345 €	360 €
from academia full	225 €	240 €
from academia reduced [3)]	105 €	120 €

[1)] No VAT requested according to § 4.22 UStG

[2)] Personal DECHEMA-, VDI-GVC-members and EFCE/EFC passport holders

[3)] First member of each academic research group pays the full academic rate, additional members pay the reduced rate (only if registration forms are sent together)

The conference ticket includes the book of abstracts, list of participants, meals and beverages during the breaks.

Conference Location

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Conference Dinner

The conference dinner will take place at the restaurant „Alte Mainmühle“ (old grain mill).
We invite you to join the Conference Dinner on Monday March 22, 2010.

Local food and wine will be served in a relaxed atmosphere. Enjoy an evening among friends and colleagues in a restaurant with the special flair of an old grain mill.

The dinner will start at 20:30. A shuttle bus will run at 20:00 from the Festung Marienberg to the restaurant „Alte Mainmühle“

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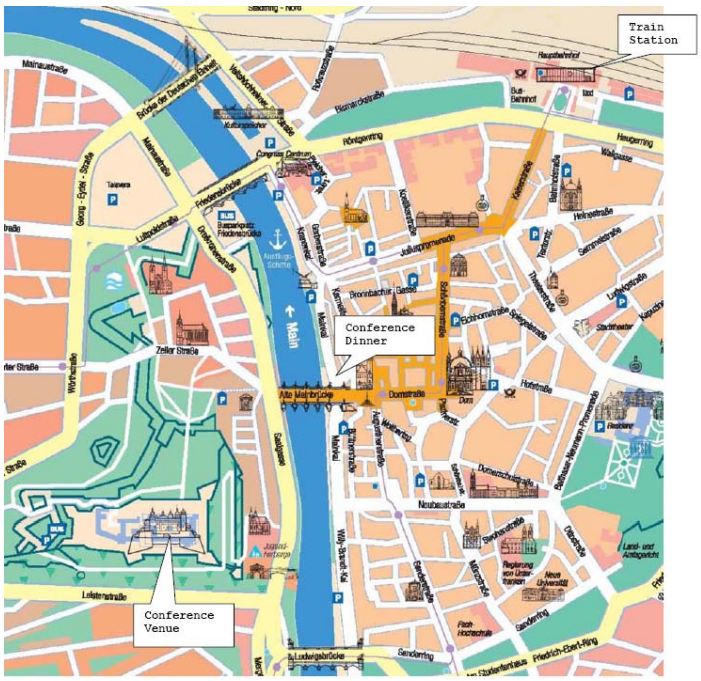

Accommodation

To reserve accommodation please contact the Congress Tourismus Wirtschaft Würzburg.
A hotel reservation form is available on the website **www.processnet.org/mol_eng_methods.**

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Organisation

The Workshop is jointly organised by

- EFCE Working Party on Thermodynamics and Transport Properties
  (Chair: I. Economou, Athens/GR and Abu Dhabi/UAE)
- ProcessNet Working Party on Molecular Modelling and Simulation for Process and Product Design
  (Chair: H. Hasse, Kaiserslautern/D)
- Local Organisation: DECHEMA e.V., Frankfurt am Main/D (R. Sass & N. Weingärtner)