ESAT

PROCESSNET
EINE INITIATIVE VON DECHEMA UND VDI-GVC

PROGRAMME

07 – 10 October 2012 · Kongresshotel Potsdam

26th European Symposium on Applied Thermodynamics

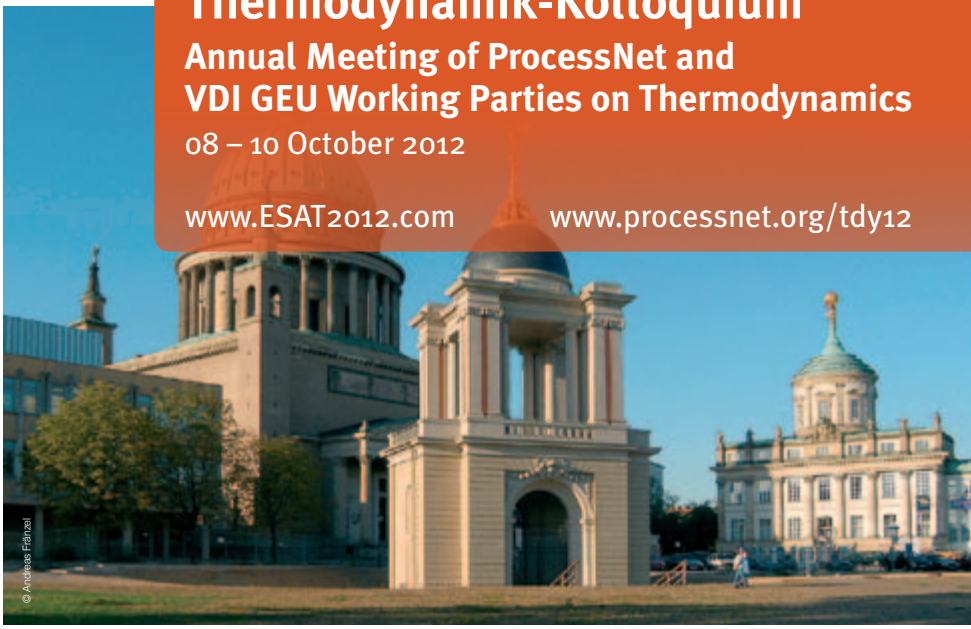
together with

Thermodynamik-Kolloquium

Annual Meeting of ProcessNet and VDI GEU Working Parties on Thermodynamics

08 – 10 October 2012

www.ESAT2012.com www.processnet.org/tdy12



DECHEMA

VDI VDI-Gesellschaft Energie und Umwelt

InPROMPT SFB/Transregio 63

ESAT

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R. Sass	Frankfurt/Main, Germany
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THERMODYNAMIK-KOLLOQUIUM

PROGRAMME COMMITTEE

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R. Span	Bochum, Germany

Sunday, October 7, 2012

	ESAT	
13:00	Registration	
15:00	Opening Ceremony	
	EFCE DISTINGUISHED LECTURE	
15:15	Klamt	
	PLENARY LECTURE	
16:15	Jaubert	
17:00	Coffee break	
	Chemical and Phase Equilibria	Polymers, Pharmaceuticals
17:30	de Hemptinne	Sarti
17:55	Dufal	Kosek
18:20	Schäfer	Chmelar
19:00-21:00	Poster Session I & Welcome Reception	

Monday, October 8, 2012

	ESAT		THERMODYNAMIK-KOLLOQUIUM	
	PLENARY LECTURES			
09:00	Span			
09:45	Kroon			
10:30	Coffee break			
	Chemical and Phase Equilibria	Polymers, Pharmaceuticals		
11:00	Paduszynski	Victorov		
11:25	Völkl	Zeiner		
11:50	Tsivintzelis	O'Connell		
12:15	Lunch		12:15	Registration
			13:00	Opening Ceremony & WATT-Award
	PLENARY LECTURES			
13:15	Ziegler			
14:00	Gilgen			
14:45	Coffee break		14:45	Coffee break
	PLENARY LECTURES			
15:30	Bardow			
16:15	Verevkin			
17:00-19:30	Poster Session II & EFCE WP-Meeting (members only)		17:00-19:30	Poster Party

Tuesday, October 9, 2012

	ESAT		THERMODYNAMIK-KOLLOQUIUM	
	PLENARY LECTURES			
09:00	Seiler			
09:45	Vrabec			
10:30	Coffee break		10:30	Coffee break
	Chemical and Phase Equilibria	Alternative Solvents (Supercritical Fluids, Ionic Liquids)	Adsorption	Thermodynamics of Energy Transformation
11:00	Secuianu	Androulaki	Knorr	Fellner
11:25	Mollerup	Maia	Fieback	Werler
11:50	Hoffmann	Domanska-Zelazna	Pflitsch	Steffen
12:15	Peper	Tuma	Morgner	Heberle
12:40	Lunch		Lunch	
	Chemical and Phase Equilibria	Alternative Solvents (Supercritical Fluids, Ionic Liquids)	Biothermodynamics	Thermodynamics of Energy Application
13:45	Wagner	Nann	Held	Kuhl
14:10	Ballerat-Busserolles	Hegel	Wolkers	Zigan
14:35	Fonseca	Francisco	Maskow	Hassel
15:00	Reiter	t.b.a.	Reschke	Löffler
15:25	Coffee break		Coffee break	
	Chemical and Phase Equilibria	Molecular and Statistical Thermodynamics	Modelling of Thermophysical Properties	Industrial Applications of Thermodynamics
16:00	Cunico	Galindo	Fayyaz	Langenbach
16:25	Rowley	Simond	Klink	Schmid
16:50	Kalies	Kontogeorgis	Arndt	Kühl
17:15	End of the conference day		End of the conference day	
17:20			General assembly of the Working Parties on Thermodynamics (members only)	
19:30			Get-together at the restaurant „Brauhaus"	
20:00	Gala dinner at the „Filmpark Babelsberg"			

Wednesday, October 10, 2012

	ESAT		THERMODYNAMIK-KOLLOQUIUM	
	PLENARY LECTURE			
08:30	Panagiotopoulos			
	Chemical and Phase Equilibria	Polymers, Pharmaceuticals	Molecular Thermodynamics	Thermodynamic Evaluation of Processes
09:20	Auger	Mannella	Vasiltsova	Frenzel
09:45	Diamantonis	Fermeglia	Koller	Dragon
10:10	Coffee break		Coffee break	
	Surfactants and Interfacial Phenomena	Molecular and Statistical Thermodynamics	Molecular Thermodynamics	Measurement of Thermophysical Properties
10:40	Peters	Economou	Windmann	Reiser
11:05	Leonhard	Sponsel	Horsch	Richter
11:30	Schrader	Wallek	Rutz	Lüddecke
11:55	Storm	Touré	Crusius	Safarov
12:20	ESAT Closing Ceremony			
12:40	Annual Meeting ProcessNet/VDI GEU Poster Award & Closing Remarks			
13:00	Lunch		13:00-14:00	WATT-Meeting (members only)
14:00	Berlin City Tour			

Sunday, October 7, 2012 — ESAT

13:00 **REGISTRATION**

15:00 **OPENING CEREMONY**
Moderation: M.E. Macedo, University of Porto/P

EFCE Distinguished Lecture in Thermodynamics and Transport Properties

Moderation: R. Dohrn, Bayer Technology Services GmbH, Leverkusen/D;
I.G. Economou, N.C.S.R. Demokritos, Aghia Paraskevi/GR

15:15 **COSMO-RS: an efficient bridge from quantum chemistry to fluid phase thermodynamics**
A. Klamt, COSMOlogic GmbH&CoKG, Leverkusen/D and University of Regensburg/D

PLENARY LECTURE

Moderation: K. Aim, ASCR, Prague/CZ; G. Sadowski, TU Dortmund/D

16:15 **Cubic equations of state: what is new since Van der Waals? Which future?**
J.N. Jaubert, R. Privat, Université de Lorraine, Nancy/F

17:00 Coffee break

Chemical and Phase Equilibria

Moderation: M.E. Macedo, University of Porto/P;
G. Maurer, University of Kaiserslautern/D

17:30 **Primary amine aqueous solutions using GC-PPC-SAFT**
J. Rozmus, J.C. de Hemptinne, P. Mougin, IFPEN, Rueil Malmaison/F

17:55 **Modelling the phase equilibria of CO_2-brine systems**
S. Dufal, A.J. Haslam, G. Jackson, A. Galindo, Imperial College London/UK

18:20 **Liquid-liquid equilibria and interfacial tension of multi-component solvent systems**
E. Schäfer, S. Enders, TU Berlin/D; G. Sadowski, TU Dortmund/D

Polymers, Pharmaceuticals

Moderation: K. Magoulas, NTUA, Athens/GR;
J. O' Connell, University of Virginia, Charlottesville/USA

17:30 **Sorption of CO_2/CH_4 mixtures in high free volume glassy polymers: experimental data and non-equilibrium modeling**
O. Vopicka, M.G. De Angelis, G.C. Sarti, University of Bologna/I; N. Du, N. Li, M.D. Guiver, National Research Council of Canada, Ottawa/CDN

17:55 **Heat transfer in nano- and micro-cellular polymeric foams**
J. Kosek, P. Ferkl, R. Pokorny, Institute of Chemical Technology Prague/CZ

18:20 **Characterization of n-pentane sorption in polystyrene**
J. Chmelar, H. Hajova, A. Nistor, J. Kosek, Institute of Chemical Technology Prague/CZ

19:00 – 21:00 **Poster Session I & Welcome Reception**

Monday, October 8, 2012 — ESAT

PLENARY LECTURES

Moderation: T.W. de Loos, TU Delft/NL;
U. Domanska-Zelazna, Warsaw University of Technology/PL

09:00 **Accurate thermodynamic-property models for CCS processes**
R. Span, J. Gernert, A. Jäger, Ruhr-Universität Bochum/D

09:45 **Nature-based deep eutectic solvents: Novel solvents for reactions and separations**
M.C. Kroon, TU Eindhoven/NL

10:30 Coffee break

Chemical and Phase Equilibria

Moderation: A. Arce, University of Santiago de Compostela/E;
J.N. Jaubert, Université de Lorraine, Nancy/F

11:00 **Capturing molecular effects on phase behavior of pure fluids and mixtures using heteronuclear PC-SAFT model: application for various alkanes**
K. Paduszynski, U. Domanska-Zelazna, Warsaw University of Technology/PL

11:25 **Design of novel solvents for CO_2 absorption by a systematic combination of a-priori calculation and process simulation**
J. Völkl, W. Arlt, University of Erlangen-Nürnberg/D

11:50 **Advanced equations of state for modeling the phase behavior of systems with supercritical, liquid or gaseous CO_2**
I. Tsivintzelis, G.M. Kontogeorgis, DTU, Lyngby/DK

Polymers, Pharmaceuticals

Moderation: R. Dohrn, Bayer Technology Services GmbH, Leverkusen/D;
A. Galindo, Imperial College London/UK

11:00 **Molecular thermodynamic modeling of gelation and phase split for polymers with strong specific interactions mixed in good solvent**
A. Victorov, St. Petersburg State University/RUS

11:25 **Aqueous two phase system based on a hyperbranched polymer**
A. Kulaguin Chicaroux, T. Zeiner, TU Dortmund/D

11:50 **Molecular structures and thermodynamics of protein stability in solution and on hydrophobic surfaces**
J. O'Connell, A. Gospodarek, E. Fernandez, University of Virginia, Charlottesville/USA

12:15 Lunch

13:15 **PLENARY LECTURES – THERMODYNAMIK- KOLLOQUIUM**

14:45 Coffee break

15:30 **PLENARY LECTURES – THERMODYNAMIK- KOLLOQUIUM**

17:00 – 19:30 **Poster Session II & EFCE WP-Meeting (members only)**

Monday, October 8, 2012 — THERMODYNAMIK-KOLLOQUIUM

12:15 **REGISTRATION**

13:00 **OPENING CEREMONY**
Moderation: G.Sadowski, TU Dortmund/D

& WATT-Award
Moderation: B. Atakan, University of Duisburg-Essen/D

PLENARY LECTURES

Moderation: R.Span, Ruhr-Universität Bochum/D

13:15 **Absorption refrigeration: relevance of the thermodynamic fundamentals for application**
F. Ziegler, TU Berlin/D

14:00 **The role of thermal power stations in the world of renewable energy**
R. Gilgen, STEAG GmbH, Essen/D

14:45 Coffee break

PLENARY LECTURES

Moderation: H. Hasse, University of Kaiserslautern/D

15:30 **Simultaneous optimization of Organic Rankine Cycle (ORC) and working fluid using PC-SAFT**
M. Lampe, A. Bardow, RWTH Aachen University/D; J. Groß, University of Stuttgart/D

16:15 **Ionic liquids and revival of solution calorimetry**
S.P. Verevkin, A.V. Yermalayeu, D.H. Zaitsau, V.N. Emelyanenko, University of Rostock/D

17:00 – 19:30 **Poster Party**

Tuesday, October 9, 2012 — ESAT

PLENARY LECTURES

Moderation: G.M. Kontogeorgis, DTU, Lyngby/DK; A. Victorov, St. Petersburg State University/RUS

09:00 **Thermodynamics and new industrial applications of hyperbranched polymers**
B. Häggman, Perstorp AB/SE; M. Seiler, Evonik Industries AG, Hanau/D

09:45 **Atomistic molecular simulations for engineering applications: methods, tools and results**
J. Vrabec, University of Paderborn/D

10:30 Coffee break

Chemical and Phase Equilibria

Moderation: T.W. de Loos, TU Delft/NL; A. Arce, University of Santiago de Compostela/E

11:00 **High-pressure phase equilibria for carbon dioxide (1) + 1-dodecanol (2) binary system**
C. Secuianu, Politehnica University of Bucharest/RO and Imperial College London/UK; V. Feroiu, D. Geana, Politehnica University of Bucharest/RO

11:25 **Thermodynamic modelling of phase equilibria in bioseparations**
J. Mollerup, PrepChrom, Klampenborg/DK

11:50 **Characterization of biological reactions accounting for thermodynamics exemplified by methyl ferulate hydrolysis**
P. Hoffmann, C. Held, G. Sadowski, TU Dortmund/D

12:15 **Sampling from fluid mixtures under high pressure: review, case study and evaluation**
S. Peper, R. Dohrn, Bayer Technology Services GmbH, Leverkusen/D

Alternative Solvents (Supercritical Fluids, Ionic Liquids)

Moderation: J.N. Jaubert, Université de Lorraine, Nancy/F; K. Magoulas, NTUA, Athens/GR

11:00 **Physical properties and heterogeneity in the dynamics of imidazolium-based [Tf_2N^-] ionic liquids**
E. Androulaki, N. Vergadou, N.C.S.R. Demokritos, Aghia Paraskevi/GR; I.G. Economou, N.C.S.R. Demokritos, Aghia Paraskevi/GR and The Petroleum Institute, Abu Dhabi/UAE

11:25 **The CPA equation of state applied to systems with ionic liquids**
F. Maia, O. Rodriguez, E. Macedo , University of Porto/P; I. Tsivintzelis, G.M. Kontogeorgis, DTU, Lyngby/DK

11:50 **Limiting activity coefficients and phase equilibria in binary systems of [BMPYR][FAP]**
U. Domanska-Zelazna, E.V. Lukoshko, M. Królikowski, Warsaw University of Technology/PL

12:15 **Gas solubility in ionic liquids: mixed gases in a pure ionic liquid and a single gas in a binary liquid mixture**
D. Tuma, BAM, Berlin/D; K. Chobanov, Stellenbosch University/ZA; J. Kumelan, Á. Pérez-Salado Kamps, G. Maurer, University of Kaiserslautern/D

12:40 Lunch

Tuesday, October 9, 2012 — THERMODYNAMIK-KOLLOQUIUM

09:00 **PLENARY LECTURES – ESAT**

10:30 Coffee break

Adsorption

Moderation: K. Schaber, KIT-Karlsruhe Institute of Technology/D

11:00 **Gibbs-adsorption isotherms of mixtures from ionic liquids with organic solvents**
A. Knorr, University of Rostock/D; M. Geppert-Rybczynska, University of Silesia, Katowice/PL; J. Safarov, A. Heintz, University of Rostock/D

11:25 **Adsorption characteristics of different solid and liquid sorbent materials**
T. Fieback, J. Rother, Ruhr-Universität Bochum/D; F. Dreisbach, Rubotherm GmbH, Bochum/D

11:50 **Novel SiC- and SiO_2-adsorbances derived from the chemical vapor infiltration of activated charcoal**
C. Pflitsch, B. Curdts, M. Helmich, D. Bathen, B. Atakan, University of Duisburg-Essen/D

12:15 **Adsorption of fluids in a mesopore: time dependent theory of hysteresis**
H. Morgner, Universität Leipzig/D

Thermodynamics of Energy Transformation

Moderation: D. Brüggemann, University of Bayreuth/D

11:00 **Selection of appropriate materials and reactor design for thermochemical energy storage (TCS)**
T. Fellner, J. Widhalm, A. Werner, F. Holzleithner, M. Haider, F. Winter, Vienna University of Technology/A

11:25 **Improvement of a plant oil stove based on experimental and numerical investigations**
M. Werler, H. Wirbser, U. Maas, B. Pritz, KIT-Karlsruhe Institute of Technology/D

11:50 **Simulation of the efficiency of a new triangle cycle with flash evaporation in a piston engine**
M. Steffen, M. Löffler, EIFER, Karlsruhe/D; K. Schaber, Institute of Technical Thermodynamics and Refrigeration, Karlsruhe/D

12:15 **Second law analysis of Organic Rankine Cycles with zeotropic fluid mixtures for geothermal power generation**
F. Heberle, D. Brüggemann, University of Bayreuth/D

12:40 Lunch

Tuesday, October 9, 2012 — ESAT

Chemical and Phase Equilibria

Moderation: J. Vrabec, University of Paderborn/D;
C. Peters, The Petroleum Institute, Abu Dhabi/UAE

13:45 **New experimental data and physico-chemical model for the solubility of carbon dioxide in aqueous solutions of monoethanolamine**
M. Wagner, I. von Harbou, J. Kim, G. Maurer, H. Hasse, University of Kaiserslautern/D

14:10 **Strategy for understanding thermophysic properties of aqueous solutions of demixing amines for CO_2 capture processes applications**
K. Ballerat-Busserolles, J.Y. Coxam, UMR CNRS Université Blaise Pascal, Aubière/F; Y. Coulier, P. Tremaine, University of Guelph/CDN

14:35 **The solubility of CO_2 and propylene oxide in polymers derived from CO_2**
J.M.S. Fonseca, R. Dohrn, A. Wolf, R. Bachmann, Bayer Technology Services GmbH, Leverkusen/D

15:00 **Development of a substitute mixture for diesel fuel**
A. Reiter, T. Wallek, P. Mair-Zelenka, A. Pfennig, M. Siebenhofer, TU Graz/A

Alternative Solvents (Supercritical Fluids, Ionic Liquids)

Moderation: U. Domanska-Zelazna, Warsaw University of Technology/PL;
G.M. Kontogeorgis, DTU, Lyngby/DK

13:45 **Thermodynamic properties for liquid-liquid extraction using ionic liquids**
A. Nann, C. Held, G. Sadowski, TU Dortmund/D

14:10 **Supercritical production and fractionation of fatty esters and monoglycerides**
P. Hegel, G. Soto, S. Pereda, G. Mabe, E. Brignole, PLAPIQUI, Bahía Blanca/RA

14:35 **Evaluation of new Deep Eutectic Solvents based on natural carboxylic acids as solvents for carbon capture**
M. Francisco, L. Zubeir, A. Van Den Bruinhorst, TU Eindhoven/NL; C. J. Peters, TU Eindhoven/NL and The Petroleum Institute, Abu Dhabi/UAE; M.C. Kroon, TU Eindhoven/NL

15:00 **t.b.a.**

15:25 Coffee break

Tuesday, October 9, 2012 — THERMODYNAMIK-KOLLOQUIUM

Biothermodynamics

Moderation: G. Sadowski, TU Dortmund/D

13:45 **Osmotic pressure of protein solutions: measurement and ePC-SAFT modeling**
C. Held, G. Sadowski, TU Dortmund/D

14:10 **Thermal fingerprinting and solvent accessibility of proteins in heart valve scaffolds**
S. Wang, Leibniz Universität Hannover/D; H. Oldenhof, University of Veterinary Medicine Hannover/D; A. Hilfiker, Hannover Medical School/D; M. Harder, Corlife GbR, Hannover/D; W.F. Wolkers, Leibniz Universität Hannover/D

14:35 **Real time analysis of metabolic and ecologic networks using calorimetry and biothermodynamics**
T. Maskow, S. Paufler, S. Oroszi, F. Buchholz, F. Mariana, Helmholtz Centre for Environmental Research - UFZ, Leipzig/D; J. Lerchner, TU Bergakademie Freiberg/D; H. Harms, Helmholtz Centre for Environmental Research - UFZ, Leipzig/D

15:00 **Modeling bio-relevant aqueous two-phase systems**
T. Reschke, C. Brandenbusch, G. Sadowski, TU Dortmund/D

Thermodynamics of Energy Application

Moderation: B. Atakan, University of Duisburg-Essen/D

13:45 **Study of transient electric field response of laminar premixed flames using PLIF and PIV techniques**
J. Kuhl, G. Jovicic, L. Zigan, A. Leipertz, University of Erlangen-Nürnberg/D

14:10 **Laser-induced fluorescence for simultaneous measurement of vapor mass fraction and temperature of a fuel spray for gasoline direct injection**
L. Zigan, J. Trost, A. Leipertz, University of Erlangen-Nürnberg/D

14:35 **Influence of the fluctuating wind and solar power input onto the thermal power plant operation**
E. Hassel, J. Nocke, S. Meinke, University of Rostock/D

15:00 **Storage devices in cold vapour cycles – improving the performance by adapting the temperature differences in the system**
M. Löffler, EIFER, Karlsruhe/D

15:25 Coffee break

Tuesday, October 9, 2012 — ESAT

Chemical and Phase Equilibria

Moderation: S.P. Verevkin, University of Rostock/D; P. Ahlström, University of Borås/S

16:00 **Consistent prediction of properties of systems with lipids**
L.P.Cunico, R. Gani, CAPEC, DTU, Lyngby/DK; R. Ceriani, UNICAMP, Campinas/BR; B. Sarup, Alfa Laval Copenhagen A/S /DK

16:25 **A systems approach for improved accuracy of thermophysical properties in the DIPPR(R) 801 database**
R. Rowley, DIPPR, Dayton/USA; W. Wilding, N. Giles, Brigham Young University, Provo/USA

16:50 **Thermodynamic interpretation of gas adsorption isotherms on highly flexible solids**
C. Reichenbach, P. Bräuer, University of Leipzig/D; M. Klauck, J. Schmelzer, G. Kalies, Dresden University of Applied Sciences/D

Molecular and Statistical Thermodynamics

Moderation: A. Victorov, St. Petersburg State University/RUS;
U. Deiters, University of Cologne/D

16:00 **Theoretical and computational developments for next generation thermodynamic modelling of complex fluids**
A. Galindo, Imperial College London/UK

16:25 **Alcanolamine-water interactions**
M.R. Simond, K. Ballerat-Busserolles, J.Y. Coxam, A.A.H. Pádua, CNRS Université Blaise Pascal, Aubière/F

16:50 **Association theories – what is possible, what is difficult, what is new?**
G.M. Kontogeorgis, I. Tsivintzelis, B. Maribo-Mogensen, DTU, Lyngby/DK

17:15 End of the conference day

20:00 **Gala dinner at the „Filmpark Babelsberg“**

Tuesday, October 9, 2012 — THERMODYNAMIK-KOLLOQUIUM

Modelling of Thermophysical Properties

Moderation: I. Smirnova, TU Hamburg-Harburg/D

16:00 **Prediction of thermo-physical properties of non-ideal mixtures with a combination of MOQUAC and cubic equations of state**
S. Fayyaz, H. Naassan, R. Bronneberg, RWTH Aachen University/D; A. Pfennig, TU Graz/A

16:25 **Density functional theory of dipolar fluids at vapour-liquid interfaces**
C. Klink, D. Weidler, G. Bauer, A. Lange, J. Groß, University of Stuttgart/D

16:50 **Modelling hydrogels with PC-SAFT**
M.C. Arndt, G. Sadowski, TU Dortmund/D

Industrial Applications of Thermodynamics

Moderation: M. Kleiber, ThyssenKrupp Uhde GmbH, Bad Soden/D

16:00 **Thermodynamic properties of branched molecules**
K. Langenbach, S. Enders, TU Berlin/D

16:25 **Application of a modern group contribution equation of state for the synthesis of thermal separation processes**
B. Schmid, J. Gmehling, DDBST GmbH, Oldenburg/D

16:50 **Efficient energy conversion by regenerative gas cycles in potential industrial application fields**
H.-D. Kühl, TU Dortmund/D

17:15 End of the conference day

17:20 **General assembly of the Working Parties on Thermodynamics (members only)**

19:30 **Get-together at the restaurant „Brauhaus“**

Wednesday, October 10, 2012 — ESAT

PLENARY LECTURE

Moderation: J. O' Connell, University of Virginia, Charlottesville/USA; S. Enders, TU Berlin/D

08:30 **Molecular simulation of phase equilibria and self-assembly**
A. Panagiotopoulos, Princeton University/USA

Chemical and Phase Equilibria

Moderation: S. Enders, TU Berlin/D; K. Leonhard, RWTH Aachen University/D

09:20 **Determination of non-bonded fractions in a series of alkanols by spectroscopy. Influence on SAFT parameters**
E. Auger, P. Tobaly, F. Volle, J.-P. Passarello, M. Dicko, LSPM CNRS Université Paris, Villetaneuse/F

09:45 **Modeling phase equilibria, thermodynamic derivative and transport properties of CO_2 mixtures**
N.I. Diamantonis, G.C. Boulougouris, D.M. Tsangaris, N.C.S.R. Demokritos, Aghia Paraskevi/GR; I.G. Economou, N.C.S.R. Demokritos, Aghia Paraskevi/GR and The Petroleum Institute, Abu Dhabi/UAE

Polymers, Pharmaceuticals

Moderation: G.C. Sarti, University of Bologna/I; K. Magoulas, NTUA, Athens/GR

09:20 **Calculation of ternary polymer solution phase diagram via compressible lattice fluid model extended to specific interactions**
G.A. Mannella, V. La Carrubba, V. Brucato, University of Palermo/I; I.C. Sanchez, University of Texas at Austin/ USA

09:45 **An integrated experimental/computational approach to the characterization of polymer-grafted silica-based polymer nanocomposites**
M. Fermeglia, P. Posocco, F. Santese, S. Pricl, University of Trieste/I; J.W. Handgraaf, Culgi B.V., Leiden/NL; M. Meyer, Jülich Centre for Neutron Science/D; O. Pravaz, University of Fribourg/CH

10:10 Coffee break

Wednesday, October 10, 2012 — THERMODYNAMIK-KOLLOQUIUM

08:30 **PLENARY LECTURE – ESAT**

Molecular Thermodynamics

Moderation: J. Vrabec, University of Paderborn/D

09:20 ***Ab initio* virial equation of state for methane**
T. Vasiltsova, J.-P. Crusius, R. Hellmann, E. Hassel, E. Bich, University of Rostock/D

09:45 **Molecular simulation of thermophysical properties of ionic liquids [EMIM][$B(CN)_4$] and [HMIM][$B(CN)_4$]**
T. Koller, M.H. Rausch, University of Erlangen-Nürnberg/D; I.G. Economou, The Petroleum Institute, Abu Dhabi/UAE; A.P. Fröba, University of Erlangen-Nürnberg/D

Thermodynamic Evaluation of Processes

Moderation: S. Will, University of Erlangen-Nürnberg/D

09:20 **Evaluation of biobased synthesis pathways based on exergy balances**
P. Frenzel, R. Hillerbrand, RWTH Aachen University/D; A. Pfennig, TU Graz/A

09:45 **Exergy calculations for a SOFC/reformer system**
M. Dragon, S. Kabelac, Leibniz Universität Hannover/D

10:10 Coffee break

Wednesday, October 10, 2012 — ESAT

Surfactants and Interfacial Phenomena

Moderation: G. Sadowski, TU Dortmund/D; T. Zeiner, TU Dortmund/D

10:40 **A theoretically based correlation for the influence parameter to calculate surface tensions using the density gradient theory**
B. Breure, C. Peters, The Petroleum Institute, Abu Dhabi/UAE

11:05 **Surface tension from PCP-SAFT-DFT and quantum mechanics**
A. von Müller, K. Leonhard, RWTH Aachen University/D

11:30 **Phase equilibria of surfactant containing systems**
P. Schrader, S. Enders, TU Berlin/D

11:55 **Micellar aqueous systems: molecular dynamics simulations for drug delivery systems**
S. Storm, T. Mehling, T. Ingram, S. Jakobtorweihen, I. Smirnova, TU Hamburg-Harburg/D; A. Panagiotopoulos, Princeton University/USA

Molecular and Statistical Thermodynamics

Moderation: I.G. Economou, N.C.S.R. Demokritos, Aghia Paraskevi/GR; J.C. de Hemptinne, IFPEN, Rueil Malmaison/F

10:40 **Molecular simulation and engineering model development for the gas-to-liquid process**
Z.A. Makrodimitri, N.C.S.R. Demokritos, Aghia Paraskevi/GR; I.G. Economou, N.C.S.R. Demokritos, Aghia Paraskevi/GR and The Petroleum Institute, Abu Dhabi/UAE; D.J.M. Unruh, Shell Global Solutions International BV, Amsterdam/NL

11:05 **Partition coefficients in systems containing large flexible surfactants: conformational study**
E. Sponsel, L. Mokrushina, W. Arlt, University of Erlangen-Nürnberg/D

11:30 **Lattice model from information theory's point of view**
T. Wallek, M. Pfleger, A. Pfennig, TU Graz/A

11:55 **Use of a new COSMO-RS based prediction method to determine the hydration number of cations**
O. Touré, C.G. Dussap, A. Lebert, Université Blaise Pascal, Aubière/F

12:20 **ESAT Closing Ceremony**
Moderation: M.E. Macedo, University of Porto/P

12:40 **Annual Meeting ProcessNet/VDI GEU – Poster Award & Closing Remarks**
Moderation: R. Span, Ruhr-Universität Bochum/D

13:00 Lunch

14:00 Berlin City Tour

Wednesday, October 10, 2012 — THERMODYNAMIK-KOLLOQUIUM

Molecular Thermodynamics

Moderation: J. Groß, University of Stuttgart/D

10:40 **Study on vapor-liquid equilibria of nitrogen + acetone and oxygen + acetone with a focus on the extended critical region**
T. Windmann, A. Köster, J. Vrabec, University of Paderborn/D

11:05 **Molecular simulation of hydrogen bonding fluids**
C. Engin, S. Reiser, M. Horsch, H. Hasse, University of Kaiserslautern/D

11:30 **Density functional and ab initio calculations for thermochemical properties and reaction path analysis of SiO_2 formation and pyrolysis**
L. Rutz, O. Deutschmann, KIT-Karlsruhe Institute of Technology/D

11:55 **Second pressure and acoustic virial coefficients and transport properties for ethylene oxide gas from an ab initio pair potential**
J.-P. Crusius, R. Hellmann, T. Vasiltsova, E. Hassel, E. Bich, University of Rostock/D

Measurement of Thermophysical Properties

Moderation: J. Gmehling, University of Oldenburg/D

10:40 **Hydrogen bonding of ethanol in supercritical mixtures with CO_2 by ^1H NMR spectroscopy and molecular simulation**
S. Reiser, N. McCann, M. Horsch, H. Hasse, University of Kaiserslautern/D

11:05 **Preliminary results of accurate (p, ρ, T, x) measurements of liquefied natural gas (LNG) using a new single-sinker densimeter**
M. Richter, R. Kleinrahm, R. Span, Ruhr-Universität Bochum/D

11:30 **CFD enhanced vibrating wire viscometry**
T. Lüddecke, Helmut-Schmidt-University - University of the Federal Armed Forces Hamburg/D; S. Kabelac, Leibniz Universität Hannover/D

11:55 **Carbon dioxide solubility in ionic liquids at high temperatures and pressures**
R. Hamidova, Azerbaijan Technical University, Baku/AZ; M. Stephan, J. Safarov, University of Rostock/D; I. Kul, Widener University, Chester/USA; A. Shahverdiyev, Azerbaijan Technical University, Baku/AZ; E. Hassel, University of Rostock/D

12:20 **ESAT Closing Ceremony**
Moderation: M.E. Macedo, University of Porto/P

12:40 **Annual Meeting ProcessNet/VDI GEU – Poster Award & Closing Remarks**
Moderation: R. Span, Ruhr-Universität Bochum/D

13:00 – 14:00 **WATT-Meeting (members only)**

Poster Session I — ESAT

P1- 1 **Avoiding thermodynamic limitations in oxidative dehydrogenation of alkanes with CO_2 as an oxidant**
K. Müller, A. Baumgärtner, L. Mokrushina, W. Arlt, University of Erlangen-Nürnberg/D

P1- 2 **Reaction equilibria in the synthesis of formylamines using CO_2 as a reactant**
K. Müller, W. Arlt, University of Erlangen-Nürnberg/D

P1- 3 **Densities, speed of sound and isentropic compressibilities of four binary mixtures of acoholes containing benzyl alcohol**
M. Papari, N. Hemmati, M.A. Faghihi, Shiraz University of Technology/IR

P1- 4 **Discussion around the paradigm of ideal mixtures with emphasis on the definition of the property changes on mixing**
R. Privat, J.N. Jaubert, Université de Lorraine – ENSIC, Nancy/F

P1- 5 **Novel approach to the reduced variables method improves phase equilibrium computations accuracy**
V. Gaganis, N. Varotsis, Technical University of Crete, Chania/GR

P1- 6 **The effect of pure components characteristic parameters on the predictions obtained by Sanchez-Lacombe equation of state**
M.A. Bashir, Aalto University, Helsinki/FIN; M.Q. Al-haj Ali, V. Kanellopoulos, E. Kokko, S. Vijay, Borealis Polymers Oy, Porvoo/FIN

P1- 7 **Precise measurement of very low vapor pressures: fewer animal testing and improved process design**
J. Fonseca, S. Peper, G. Olf, R. Dohrn, Bayer Technology Services GmbH, Leverkusen/D

P1- 8 **Key issues in the measurement of VLE with balanced-pressure head-space gas chromatography**
P. Luis, B. Van der Bruggen, Katholieke Universiteit Leuven/B

P1- 9 **Phase equilibrium calculations with quasi-Newton methods**
D. Nichita, M. Petitfrere, University of Pau/F

P1- 10 **Suitability of deep eutectic solvents (organic salt + natural carboxylic acid mixtures) for lignocellulosic biomass processing**
M. Francisco, A. Van Den Bruinhorst, M.C. Kroon, TU Eindhoven/ NL

P1- 11 **Dew point predictions of natural gases**
E. Panteli, G. Pappa, V. Louli, E. Voutsas, NTUA, Athens/GR; E. Solbraa, E. Skouras, Statoil ASA, Trondheim/N

P1- 12 **Predicting protein solubility in aqueous solutions based on the second osmotic virial coefficient** M. Herhut, TU Dortmund/D

P1- 13 **Application of the NRTL-PR model to the prediction of solid-supercritical fluid equilibria and high pressure excess enthalpies**
J. Escandell, E. Neau, Aix-Marseille University/F

POSTER PROGRAMME

Poster Session I — ESAT

P1- 14 **Density measurements under pressure of 2-butanol at temperatures up to 393.15 K and at pressures up to 70 MPa.**
M. Dakkach, Abdelmalek Essaâdi University, Tetouan/MA; F. Aguilar, F. Alaoui, E. Montero, Universidad de Burgos/E

P1- 15 **New oxygenated additives in bio-fuels: excess enthalpies of mixtures 1-propanol + methylcyclohexane or + 1-hexene at 298.15 and 313.15 K.**
F. Alaoui, F. Aguilar, M.J. Gonzalez-Fernandez, Universidad de Burgos /E; A. El Amarti, Abdelmalek Essaâdi University, Tetouan/MA; E. Montero, Universidad de Burgos/E

P1- 16 **Solubility of carbohydrates and sugar alcohols in ionic liquids based on dicyanamide anion – measurements and thermodynamic modeling**
A. Carneiro, O. Rodríguez, E.A. Macedo, University of Porto/P

P1- 17 **Molecular-level vapour-liquid equilibrium algorithm for dew-points in multicomponent mixtures and application in the chemical industry**
M. Skvorova, I. Nezbeda, J.E. Purkinje University, Usti nad Labem/CZ; W.R. Smith, University of Guelph/CDN

P1- 18 **Equilibrium studies on the separation of formic acid from aqueous solutions by bulk liquid membrane technique**
M. Bilgin, B. Baslioglu, Istanbul University/TR

P1- 19 **Phase behavior of mixed monolayers of rage gases on graphite**
A. Patrykiejew, Maria Curie-Sklodowska University, Lublin/PL

P1- 20 **Rapid determination of multicomponent diffusion using microfluidics**
C. Blesinger, S. Yalcin, C. Pauls, A. Bardow, RWTH Aachen University/D

P1- 21 **High pressure phase behavior data of selected ternary systems containing organics + ionic liquid + carbon dioxide**
S. Kazemi, TU Delft/NL; C.J. Peters, TU Delft/NL and TU Eindhoven/NL and The Petroleum Institute, Abu Dhabi/UAE; M.C. Kroon, TU Eindhoven/NL; M. Francisco, TU Eindhoven/NL

P1- 22 **Behaviour of ethylenglycol and glycerine as entrainers for the extractive distillation of azeotropic mixture ethanol + water**
J. Pla-Franco, S. Loras, E. LLadosa, J.B. Montón, University of Valencia, Burjassot/E

P1- 23 **Liquid-liquid equilibria study of 4-methyl-2-pentanone + 2-propanol + water system**
J. Pla-Franco, A. Cháfer, J. de la Torre, E. Lladosa, University of Valencia, Burjassot/E

P1- 24 **A rapid and robust method for solving the Rachford-Rice equation using convex transformations**
D. Nichita, University of Pau/F; C. Leibovici, CFL Consultant, Pau/F

P1- 25 **Ternary phase equilibria of (water – acetic acid – ethyl heptanoat) liquid systems at several temperatures**
Ç. Demirel, S. Çehreli, Istanbul University/TR

Poster Session I — ESAT

P1- 26 **Process simulation: the need for an advanced thermophysical calculation server**
O. Baudouin, S. Déchelotte, A. Vacher, ProSim SA, Labege/F; B. Wincure, ProSim, Inc., Philadelphia/USA

P1- 27 **The effect of SDS on the electrokinetic curves at various solid-to-liquid ratios**
M. Kosmulski, E. Mączka, Lublin University of Technology/PL

P1- 28 **Measurements and modeling of phase equilibrium of systems containing polar chemicals**
M. Frost, N. von Solms, E.H. Stenby, G.M. Kontogeorgis, DTU, Lyngby/DK; E. Solbraa, Statoil ASA, Trondheim/N;

P1- 29 **The thermodynamic analogy of processes**
G. Kalies, Dresden University of Applied Sciences/D; P. Bräuer, University of Leipzig/D

P1- 30 **Phase behavior and interfacial tension of gas mixtures at low temperatures and elevated pressure**
S. Knauer, P.T. Jaeger, TU Hamburg-Harburg/D; G.O. Amezquita, TU Berlin/D

P1- 31 **Measurements of vapour–liquid equilibria in systems consisting of compounds with isopropyl group**
J. Pavlíček, G. Bogdanić, I. Wichterle, ASCR, Prague/CZ

P1- 32 **High temperature vapour-liquid equilibria of water alcohol mixtures**
A. Cristino, S. Rosa, Lisbon University/P; P. Morgado, E.J.M. Filipe, A.M.F. Palavra, Instituto Superior Técnico, Lisbon/P; A. Galindo, Imperial College London/UK; C.A. Nieto de Castro, Lisbon University/P

P1- 33 **Phase equilibria, excess enthalpy and modelling of pyrrole solutions with benzene, cyclohexane and alcohols**
U. Domanska-Zelazna, M. Zawadzki, Warsaw University of Technology/PL

P1- 34 **Prediction and experimental determination of VLE in systems containing water, cyclohexane/methylcyclohexane, aniline and cyclohexylamine**
M. Klauck, R. Metasch, T. Jasinowski, G. Kalies, J. Schmelzer, Dresden University of Applied Sciences/D

P1- 35 **Liquid mixtures involving fluorinated alcohols: the equation of state (p, r, T, x) of (ethanol + trifluoroethanol) experimental and simulation**
P. Duarte, D. Rodrigues, M. Silva, P. Morgado, E.J.M. Filipe, Instituto Superior Técnico, Lisbon/P; L. Martins, Instituto Superior Técnico, Lisbon/P and Universidade de Évora, Sé/P

P1- 36 **Liquid mixtures involving fluorinated alcohols: surface tension of (trifluoroethanol + ethanol), (trifluoroethanol + propanol) and (trifluoroethanol + butanol)**
M. Teixeira, P. Morgado, E.J.M. Filipe, Instituto Superior Técnico, Lisbon/P

P1- 37 **Fluid phase equilibria: consistency tests and experimental data correlation deficiencies**
A. Marcilla, M.M. Olaya, J.A. Reyes-Labarta, M.D. Serrano, University of Alicante/E

P1- 38 **Atomistic modelling of protein superabsorbents**
E. Erdtman, University of Borås/S; T. Gebäck, University of Borås/S and Chalmers University of Technology, Göteborg/S; P. Ahlström, University of Borås/S

Poster — THERMODYNAMIK-KOLLOQUIUM

T1 **Van't Hoff's equation for isothermal phase equilibria – a forgotten relation?**
U. Deiters, University of Cologne/D

T2 **Influences on the accuracy for temperature measurements using thermocouples**
A. Sielaff, F. Crößmann, P. Stephan, TU Darmstadt/D

T3 **Optical Flow Method as an alternative to Particle Image Velocimetry for easy analysing biofuel spray velocity fields**
S. Lorenz, University of Bayreuth/D; J. Goldlücke, Goldlücke Ingenieurleistungen, Erlangen/D; S. Lehmann, W. Mühlbauer, D. Brüggemann, University of Bayreuth/D

T4 **Solubility of CO and synthesis gas in liquid solvents for hydroformylation reactions**
C. Vogelpohl, C. Brandenbusch, G. Sadowski, TU Dortmund/D

T5 **Systematic model-based design of experiments for the data reduction of liquid-liquid equilibria**
D. Dechambre, A. Bardow, K. Leonhard, RWTH Aachen University/D; L. Greiner, DECHEMA-Forschungsinstitut, Frankfurt am Main/D

T6 **Thermophysical properties of synthetic geothermal fluids**
U. Hoffert, H. Milsch, Helmholtz Centre Potsdam GFZ German Research Centre for Geosciences, Potsdam/D

T7 **Density and speed of sound of Kura River waters of Azerbaijan**
S. Babayeva, Azerbaijan State Oil Academy, Baku/AZ; G. Aliyeva, Azerbaijan Technical University, Baku/AZ; J. Safarov, University of Rostock/D; A. Shahverdiyev, Azerbaijan Technical University, Baku/AZ; E. Hassel, University of Rostock/D

T8 **The combustion and vaporization thermodynamics of biodiesel**
D.H. Zaitsau, S. P. Verevkin, V. N. Emelyanenko, University of Rostock/D

T9 **A study of the vapour-liquid equilibrium of ferrocene in some organic solvents using spectroscopic methods**
M.A. Siddiqi, M. Kimoto, K. Haroun, University of Duisburg-Essen/D; P. Reddy, University of KwaZulu-Natal, Durban/ZA; B. Atakan, University of Duisburg-Essen/D

T10 **An apparatus for the gravimetric preparation of gas mixtures**
M. Schäfer, R. Wegge, M. Richter, R. Span, Ruhr-Universität Bochum/D

T11 **Rare earth doped alumina coatings for surface temperature measurements**
D. Stenders, I. Kayacan, C. Eckert, B. Atakan, C. Pflitsch, University of Duisburg-Essen/D

T12 **Speed of sound of siloxanes as workings fluids in Organic Rankine Cycles**
F. Dubberke, J. Vrabec, University of Paderborn/D

T13 **CoMT-CAMD: simultaneous process and solvent design using PCP-SAFT applied to CO_2 capture**
M. Stavrou, University of Stuttgart/D; A. Bardow, RWTH Aachen University/D; J. Groß, University of Stuttgart/D

Poster — THERMODYNAMIK-KOLLOQUIUM

T14 **HelmholtzMedia – a fluid property library for dynamic simulation**
M. Thorade, A. Saadat, Helmholtz Centre Potsdam GFZ German Research Centre for Geosciences, Potsdam/D

T15 **Morphological analysis of self-assembled diblock copolymer structures in dissipative particle dynamics simulations**
J. Skvor, Z. Posel, J. E. Purkinje University in Usti nad Labem/CZ

T16 **Numerical computation of real gas CH_4/O_2 counterflow diffusion flames using OpenFOAM**
H. Müller, S. Pohl, M. Jarczyk, M. Pfitzner, Universität der Bundeswehr München, Neubiberg/D

T17 **Development of a Helmholtz energy based empirical model for thermodynamic properties of ethanol-water mixtures**
T. Wiens, R. Span, Ruhr-Universität Bochum/D; E. Lemmon, National Institute of Standards and Technology, Boulder/USA

T18 **Nonadditive potentials for molecular simulations of thermodynamic properties**
T. Vasiltsova, B. Jäger, E. Hassel, E. Bich, University of Rostock/D

T19 **Thermodynamic properties of argon from the ab initio virial equation of state**
B. Jäger, University of Rostock/D

T20 **Thermodynamic properties of an ionic liquid via molecular dynamics simulation**
T. Köddermann, M. Hülsmann, K. Kirschner, D. Reith, Fraunhofer Institute SCAI, Sankt Augustin/D

T21 **Molecular simulation of thermodynamic properties and an equation of state for the Lennard-Jones model fluid**
M. Thol, Ruhr-Universität Bochum/D; G. Rutkai, University of Paderborn/D; R. Span, Ruhr-Universität Bochum/D; J. Vrabec, University of Paderborn/D

T22 **Examination of COSMO-RS approximations with intermolecular surface contact statistics from MD simulations**
R.E. Isele-Holder, B.D. Rabideau, A.E. Ismail, RWTH Aachen University/D

T23 **Spline based interpolation of the two phase region of binary mixtures using multiparameter equations of state**
C. Schulze, TLK-Thermo GmbH, Braunschweig/D; J. Köhler, TU Braunschweig/D

T24 **Analysis of a perturbational approach for electrolyte solutions**
F. Drunsel, W. Zmpitas, J. Groß, University of Stuttgart/D

T25 **Prediction of liquid-liquid equilibria of nitrogen + ethane with a molecular model that was adjusted to vapor-liquid equilibria**
S. Eckelsbach, J. Vrabec, University of Paderborn/D

POSTER PROGRAMME

Poster — THERMODYNAMIK-KOLLOQUIUM

T26 **An accurate and consistent description of hydrates in $H_2O + CO_2$ mixtures**
A. Jäger, Ruhr-Universität Bochum/D; V. Vinš, Institute of Thermomechanics AS CR, v. v. i., Prague/CZ; J. Gernert, R. Span, Ruhr-Universität Bochum/D; J. Hrubý, Institute of Thermomechanics AS CR, v. v. i., Prague/CZ

T27 **Particulate emissions of a single cylinder diesel engine operating on biodiesel blends under different load conditions with EGR**
W. Mühlbauer, U. Leidenberger, S. Lorenz, S. Lehmann, D. Brüggemann, University of Bayreuth/D

T28 **Semiclassical approach to model quantum fluids combining discrete pair potential method and the SAFT-VRQ approach**
V.M. Trejos Montoya, A. Gil-Villegas, Guanajuato University/MEX

T29 **Calculation of liquid-liquid and liquid-solid equilibria of polymer solution using lattice cluster theory**
J. Sailer, K. Langenbach, S. Enders, TU Berlin/D

T30 **Detection of the biologic energy system's quantized structure by calculation of exergetic and anergetic reaction data**
R. Radebold, RADEBOLD Ingenieurbüro, Berlin/D

T31 **Survey on the methods of methane gas liquefaction and economical justification of LNG production by Claude cycle**
M. Rahmanzade, A. Moradi, S. Soltaninejad, M. Kazemiranjbar, Shahid Bahonar University of Kerman/IR

T32 ***In-situ* gas analysis**
J. Moeller, T. Fieback, R. Span, Ruhr-Universität Bochum/D

T33 **Energetic optimisation of the waste incineration plant Rostock – a thermodynamic approach using process simulation and experiments**
M. Hübel, J. Nocke, E. Hassel, University of Rostock/D

T34 **Property libraries for working fluids for calculating heat cycles, boilers, turbines, heat pumps and refrigeration processes**
H.-J. Kretzschmar, I. Stoecker, M. Kunick, S. Herrmann, University of Applied Sciences Zittau/Görlitz/D

T35 **Simulation of an exhaust-heat driven Rankine Cycle**
J. Wiedemann, R. Span, Ruhr-Universität Bochum/D

T36 **Modified adsorbents derived from charcoal: solvent adsorption studies**
C. Pflitsch, B. Curdts, M. Helmich, D. Bathen, B. Atakan, University of Duisburg-Essen/D

Poster — THERMODYNAMIK-KOLLOQUIUM

T37 **Investigation of fluid phase equilibria for the oxidation of cyclohexane in carbon dioxide expanded liquids from experiment, molecular simulation, the Peng-Robinson EOS and COSMO-SAC**
T. Merker, University of Kaiserslautern/D; C.-M. Hsieh, University of Paderborn/D; S.-T. Lin, National Taiwan University, Taipei/TW; H. Hasse, University of Kaiserslautern/D; J. Vrabec, University of Paderborn/D

T38 **Modifications of the h-O diagram**
C. Pels Leusden, Beuth University of Applied Sciences Berlin/D

T39 **Absorption heat transformer with the working pair ionic liquid – water**
N. Merkel, C. Römich, P. Meysel, M. Gleiß, KIT-Karlsruhe Institute of Technology/D; T.J.S. Schubert, Ionic Liquids Technologies GmbH, Heilbronn/D; K. Schaber, KIT – Karlsruhe Institute of Technology/D

T40 **Energetic, environmental and economic issues of the district heating of the Hanseatic City of Rostock**
M. Theile, University of Rostock/D

T41 **Methane conversion at elevated pressures: experiment and simulation**
F. Sen, U. Bergmann, B. Atakan, University of Duisburg-Essen/D

T42 **Ecological plant oil stove for developing and emerging countries**
M. Werler, H. Wirbser, U. Maas, KIT-Karlsruhe Institute of Technology/D

T43 **Analysis of Organic Rankine Cycle with regard to the chemical class of the working fluid**
M. Preißinger, D. Brüggemann, University of Bayreuth/D

T44 **EGR-Cooling – A challenge to fulfill future emission regulations for medium speed engines**
M. Sturm, C. Rickert, Caterpillar Motoren GmbH & Co. KG, Kiel/D; D. Krauß, GEA Luftkühler GmbH, Herne/D; M. Reißig, M. Drescher, FVTR GmbH, Rostock/D

T45 **Energy-efficient generation of compressed air from waste heat**
N. Schröder, H.-D. Kühl, TU Dortmund/D

T46 **Energetic estimation of a solar powered cogeneration system for single- and multi-family houses**
P. Petr, T. Alpögger, J. Köhler, TU Braunschweig/D; W. Tegethoff, TLK Thermo GmbH, Braunschweig/D

T47 **Exergy analysis within process simulation software to enhance process energy management**
P. Baudet, O. Baudouin, S. Déchelotte, ProSim SA, Labege/F; P. Floquet, A. Ghannadzadeh, X. Joulia, R. Thery-Hetreux, Université de Toulouse – CNRS/F; B. Wincure, ProSim, Inc., Philadelphia/USA

T48 **On the history of ejectors and ejector refrigerators**
J. Fischer, University of Natural Resources and Life Sciences, Vienna/A

Poster Session II — ESAT

P2- 1 **High pressure solubility of carbon dioxide in non-fluorinated phosphonium-based ionic liquids**
M. Ramdin, T.J.H. Vlugt, T.W. de Loos, TU Delft/NL

P2- 2 **Experimental study and modeling of methane hydrate formation induction time in the presence of ionic liquids**
J. Javanmardi, A. Rasoolzadeh, Shiraz University of Technology /IR; A. Eslamimanesh, A.H. Mohammadi, MINES ParisTech/F

P2- 3 **Phase equilibria study of the binary systems (N-hexylisoquinolinium thiocyanate ionic liquid + organic solvent, or water)**
M. Królikowska, M. Karpinska, M. Zawadzki, Warsaw University of Technology/PL

P2- 4 **Modeling Imidazolium-based Ionic Liquids with ePC-SAFT**
X. Ji, LTU, Lulea/S; C. Held, G. Sadowski, TU Dortmund/D

P2- 5 **Heat capacities and excess enthalpies of the {N-octylisoquinolinium thiocyanate ionic liquid + water} binary systems**
M. Królikowska, M. Królikowski, J. Antonowicz, Warsaw University of Technology/PL

P2- 6 **Synthesis and physicochemical properties of a novel nicotinic acid derivatives ionic liquids**
M. Królikowski, M. Zawadzki, U. Domanska-Zelazna, K. Skiba, Warsaw University of Technology/PL

P2- 7 **Limiting activity coefficients of various solutes in piperidinium cation-based ionic liquids: measurements and LSER calculations**
K. Paduszynski, U. Domanska-Zelazna, Warsaw University of Technology/PL

P2- 8 **A generalized correlation for solid solubilities in supercritical carbon dioxide based on the SRK EoS**
K. Mulia, A. Chrisnandy, Universitas Indonesia, Depok/RI

P2- 9 **Study of phase behavior of trihexyl(tetradecyl)phosphonium bis(trifluoromethylsulfonyl)imide ionic liquid for enhanced oil recovery**
S. Lago, E. Rodil, A. Soto, A. Arce, University of Santiago de Compostela/E

P2- 10 **Extractive and oxidative desulfurisation of fuels with the ionic liquid [$h^{2,4}$mmpy][NTf_2]**
B. Rodríguez-Cabo, M. Francisco, A. Soto, A. Arce, University of Santiago de Compostela/E

P2- 11 **Mixed ionic liquids ([CnC2im][$EtSO_4$] + [C2C1im][NTf_2]) for absorption of carbon dioxide**
A.M. Pinto, H. Rodríguez, A. Soto, A. Arce, University of Santiago de Compostela/E

P2- 12 **Thermophysical characterisation of mixtures of ionic liquids: [C2C1im][NTf_2] + [CnC2im][$EtSO_4$]**
A.M. Pinto, H. Rodríguez, A. Soto, A. Arce, University of Santiago de Compostela/E

P2- 13 **Molecular dynamics simulations of ionic liquid/water mixtures: water concentration effects**
A. Niazi, B. Rabideau, A.E. Ismail, RWTH Aachen University/D

Poster Session II — ESAT

P2- 14 **High-pressure phase behavior of 1-butyl-1-methylimidazolium nonafluorobutane sulfonate and CO_2 binary system**
S.K. Hong, Y. Park, Hongik University, Sejong/ROK; D.M. Pore, Shivaji University, Kolhapur/IND

P2- 15 **The study of excess enthalpies of the binary mixtures {N-octylisoquinolinium bis{(trifluoromethyl)sulfonyl}imide + organic solvent}**
M. Królikowski, M. Zawadzki, U. Domanska-Zelazna, Warsaw University of Technology/PL

P2- 16 **Heat capacities of bis(trifluoromethylsulfonyl)imide quaternary ammonium ionic liquids and excess properties of their mixtures with methanol**
K. Machanová, M. Bendová, Z. Wagner, K. Aim, ASCR, Prague/CZ; J. Troncoso, Universade de Vigo, Ourense/E

P2- 17 **Sorption in polyolefins: equilibria, diffusion and morphology**
J. Chmelar, A. Zubov, J. Kosek, Institute of Chemical Technology, Prague/CZ

P2- 18 **Phase transition of N-isopropylacrylamide nanometer-sized gel particles in aqueous polymer solutions**
S.M. Kim, Y.C. Bae, Hanyang University, Seoul/ROK

P2- 19 **Sorption and diffusion of gases and vapors in poly (exo,endo-3,4-bis(trimethylsilyl) tricyclononene)**
O. Vopicka, M.G. De Angelis, G.C. Sarti, University of Bologna /I; Y. Yampolskii, E. Finkelshtein, Russian Academy of Sciences, Moscow/RUS

P2- 20 **Development and application of a PPPM method for long-range dispersion interactions**
R.E. Isele-Holder, A.E. Ismail, RWTH Aachen University/D

P2- 21 **Study of aggregative behavior of surfactants in "water + glycerol" media for optimizing stabilization of carbon nanotubes dispersions**
A.V. Venediktova, A.Y. Vlasov, X.R. Savchuk, N.A. Smirnova, St.Petersburg State University/RUS

P2- 22 **What can we learn from putting speed of sound data into the universal constants regression in PC-SAFT?**
X. Liang, G.M. Kontogeorgis, DTU, Lyngby/DK

P2- 23 **Phase equilibria modeling of glycols and derivatives by group contribution**
J. Merino, T.M. Soria, F.A. Sanchez, S.B. Bottini, S. Pereda, PLAPIQUI, Bahía Blanca/RA

P2- 24 **The role of intermolecular interactions for phase miscibility in polymer solutions: molecular simulations and thermodynamic modeling**
S.Y. Oh, Y.C. Bae, Hanyang University, Seoul/ROK

P2- 25 **Thermodynamics and structure of fluids of smeared charge particles: the hypernetted-chain closure**
A.L. Nikolaeva, A.Y. Vlasov, St.Petersburg University/RUS

POSTER PROGRAMME

Poster Session II — ESAT

P2- 26 **Aspects of the stability of biaxial phase in ternary nematic mixtures of hard axially-symmetric particles**
E.P. Sokolova, A.Y. Vlasov, St.Petersburg University/RUS

P2- 27 **An extended SAFT equation of state for polar, non-polar fluids: applicability to hydrogen bonding of water and alcohol system**
Y.G. Kim, Y.C. Bae, Hanyang University, Seoul/ROK

P2- 28 **Adsorption of ions on surfaces modified by tethered layers of polyelectrolytes: a density-functional approach**
S. Sokolowski, M. Borowko, A. Patrykiejew, Maria Curie-Sklodowska University, Lublin/PL

P2- 29 **End-grafted chain layers immersed into different solvents – a density functional study**
M. Borowko, S. Sokolowski, T. Staszewski, Maria Curie-Sklodowska University, Lublin/PL

P2- 30 **Polymer brushes: solvent size effects**
M. Borowko, S. Sokolowski, T. Staszewski, Maria Curie-Sklodowska University, Lublin/PL

P2- 31 **Adsorption from a monomer-oligomer solution on the surface modified with attached short chains**
T. Staszewski, M. Borowko, S. Sokolowski, Maria Curie-Sklodowska University, Lublin/PL

P2- 32 **Phase equilibrium predictions in ionic liquids mixtures with UNIFAC and COSMO-RS**
E. Alevizou, K. Magoulas, E. Voutsas, NTUA, Athens/GR

P2- 33 **New viscosity-surface correlations for propane, n-butane, and isobutane using a structure-optimisation method**
S. Herrmann, University of Applied Sciences Zittau/Görlitz/D; E. Vogel, E. Hassel, University of Rostock/D; R. Span, Ruhr-Universität Bochum/D

P2- 34 **Modelling the permittivity of electrolyte solutions in water and mixed solvents**
J. Mollerup, PrepChrom, Klampenborg/DK

P2- 35 **Molecular dynamics simulations study on chiral room-temperature ionic liquids**
M. Lísal, J.E. Purkinje University, Usti nad Labem/CZ; Z. Chvál, University of South Bohemia, České Budějovice/CZ; J. Storch, P. Izák, K. Aim, ASCR, Prague/CZ

P2- 36 **Heat transfer and crystallization in infrared irradiated semi-crystalline polymer composites**
M. Fischlschweiger, A. Stock, D. Mungenast, S. Picheta, G. Hartung, P. Egger, ENGEL Austria GmbH, St. Valentin/A

P2- 37 **Applying the PPC-SAFT EOS to multifunctional oxygenated compounds and their mixtures**
L. Grandjean, IFPEN, Rueil Malmaison/F; E. Auger, LSPM, Villetaneuse/F; R. Lugo, A. Di Lella, IFPEN, Rueil Malmaison/F; P. Tobaly, J.-P. Passarello, LSPM, Villetaneuse/F; J.-C. de Hemptinne, IFPEN, Rueil Malmaison/F

NOTES

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