



29th European Symposium on Applied Thermodynamics – ESAT 2017
May 18-21, 2017, Radisson Blu Hotel, Bucharest, ROMANIA

Poster Program

Phase equilibria & transport properties (experimental & modelling)

- P1 *Phase equilibria, thermophysical and excess thermodynamic properties for model IL + classical solvent systems*
Mariana Teodorescu, Vlad Tudor Popa
- P2 *Phase equilibria study and modelling of the Deep Eutectic Solvents*
Marek Królikowski, Aleksandra Lipińska
- P3 *Solubilities for {LiBr (1) + water (2) + IL (3)} ternary systems at various temperatures and compositions*
Marta Królikowska
- P4 *Thermodynamic and transport properties of aqueous mixtures of carboxylic-based ionic liquids*
Marta Królikowska, Maciej Zawadzki
- P5 *Hydrate equilibrium measurements of the ternary CH₄ + CO₂ + H₂O system*
Panagiotis Kastanidis, George E. Romanos, **Ioannis G. Economou**, Athanassios K. Stubos, Ioannis N. Tsimpanogiannis
- P6 *Vapour-liquid equilibria in ternary systems containing cyclohexanol*
Mandy Klauck, Thomas Hähnel, Sandra Richter, Christian Nowka, Jürgen Schmelzer, Grit Kalies
- P7 *Calculation of the solubility constants of hydrated geological solid phases involving aluminium, sulfate and hydroxyl species*
Christelle Goutaudier, Angélique Teyssier, Vincent Lagneau, Jean-Michel Schmitt, Jean-Jacques Counieux
- P8 *Assessing entropy scaling of transport properties of mixtures using Molecular Simulations*
Matthias Fischer, Oliver Lötgering-Lin, Joachim Groß
- P9 *Phase equilibria of limonene with p-cymene, indane, butylbenzene and 1,2,3-trimethylbenzene*
Rajesh Gowda, A. Cédric Kouakou, **Cara E. Schwarz**
- P10 *Comparing the Holistic Predictive Strength of Different SAFT Variants*
Jamie T. Cripwell, Sonja A.M. Smith, Cara E. Schwarz, **Andries J. Burger**
-



29th European Symposium on Applied Thermodynamics – ESAT 2017
May 18-21, 2017, Radisson Blu Hotel, Bucharest, ROMANIA

Poster Program

Phase equilibria & transport properties (experimental & modelling)

- P11** *Evaluation of Cubic-Plus-Association parameterization for monoethylene glycol*
Francois Kruger, Nicolas von Solms, Georgios Kontogeorgis
- P12** *Modeling of mixtures containing alcohols and light gases with water and salts by means of the NRTL-PRA model*
Evelyne Neau, **Christophe Nicolas**
- P13** *Experimental study of complete inhibition region of methane hydrate formation in the presence of PVP and PVCap aqueous solutions*
Mohamad Roostaei, **Jafar Javanmardi**, Bahman Tohidi
- P14** *Addition of the alkyne groups to the E-PPR78 model*
Xiaochun Xu, Romain Privat, Philippe Arpentinier, Jean-Noël Jaubert
- P15** *Variation of the Watson characterization factor for oil with polar and aromatic compounds*
Vahur Oja, Oliver Järvik, Zachariah S. Baird, Rivo Rannaveski
- P16** *15 years with the development of predictive cubic equations of state: what have we learnt?*
Jean-Noël Jaubert, Romain Privat
- P17** *Efficient determination of liquid-liquid equilibria using microfluidics and Raman microspectroscopy*
Julia Thien, Christine Peters, Thorsten Brands, Hans-Jürgen Koß and André Bardow
- P18** *An improved apparatus for vapor–liquid equilibria measurement in polymer + solvent systems at higher temperatures*
Jan Pavlíček, Grozdana Bogdanić, **Ivan Wichterle**
- P19** *Effect of enthalpy prediction on Katz diagrams in allowable pressure drop across a throttle valve for avoiding gas hydrate formation*
Mohamadmostafa Owji, **Jafar Javanmardi**, Bahman Tohidi
- P20** *Equation of state modeling of solid – liquid – gas equilibrium of asymmetric binary mixtures of methane with heavy n-alkanes*
Varvara S. Samoili, **Ilias K. Nikolaidis**, Epaminondas C. Voutsas, Ioannis G. Economou



29th European Symposium on Applied Thermodynamics – ESAT 2017
May 18-21, 2017, Radisson Blu Hotel, Bucharest, ROMANIA

Poster Program

Phase equilibria & transport properties (experimental & modelling)

- P21 *A reference database for the comparison and validation of thermodynamic models*
Yohann Le Guennec, Romain Privat, Jean-Noël Jaubert
- P22 *Investigation of the thermophysical properties of binary system CO₂ and Hydro-fluoro-olefins*
Pierre-Arnaud Artola, **Bernard Rousseau**, Rémi Fauve, Elise El Ahmar, Céline Houriez, Christophe Coquelet
- P23 *Liquid–vapor and solid–fluid equilibria for the system CO₂ - nC₁₇ at high pressure*
Jérôme Pauly, Jean-Luc Daridon, **Dan Vladimir Nichita**
- P24 *High pressure data and PC-SAFT modeling of Amines*
Hosseinali Zarei, Rokhsareh Mohammadkhani, Ameneh Paknejad
- P25 *The state-of-the-art of available thermodynamic models for N₂-O₂-Ar mixtures*
Silvia Lasala, Romain Privat, Jean-Noël Jaubert, Philippe Arpentinier
- P26 *The thermodynamics of mixtures characterized by discontinuous critical points loci*
Silvia Lasala, Romain Privat, Jean-Noël Jaubert
- P27 *Vapor-liquid equilibrium for the systems ethanol + frying oil biodiesel*
Pollyana M. Kalvelage, **Allan A. Albuquerque**, Luiz Stragevitch, António A. C. Barros, Sávio L. Bertoli
- P28 *Liquid–liquid equilibrium for mixtures of n-hexadecane + xylene + pyrene + sulfolane*
Flávio M. P. Lopes, **Allan A. Albuquerque**, Luiz Stragevitch
- P29 *Separation of alkyl-benzenes from methyl cyclohexane using 1-ethyl-3-methylimidazolium bis{(trifluoromethyl)sulfonyl}imide*
Elena Gracsová, Karel Řehák, Lenka Karolyová
- P30 *LLE description of ternary systems containing ionic liquids*
Elena Gracsová, Pavol Steltenpohl



29th European Symposium on Applied Thermodynamics – ESAT 2017
May 18-21, 2017, Radisson Blu Hotel, Bucharest, ROMANIA

Poster Program

Phase equilibria & transport properties (experimental & modelling)

- P31** *VLE description of ternary systems containing ionic liquids*
Elena Graczová, Pavol Steltenpohl
- P32** *CO₂ Capture from Flue Gas Using Gas Hydrate Technology: A Process Design*
Olamide H. Animasahun, Mohammad Ahmed Ali, M. Naveed Khan, Carolyn A. Koh, **Cor J. Peters**
- P33** *Analisis of viscosity of the binary system n-octane + 1-alkanol*
Santiago Castelo, Ana Gayol, **Marta M. Mato**, Manuel Martínez Piñeiro, José Luis Legido
- P34** *Thermodynamic Aspects of Cobaltocene Mass Transfer in CH₃CN*
Diana Adela Berinde, **Eleonora Mihaela Ungureanu**, Oana Ciocîrlan, Magda R. Bujduveanu
- P35** *Volumetric properties of the D2EHPA – o-xylene – di-(2-ethylhexyl)phosphate lanthanide solutions*
Svetlana V. Kurdakova, Taisiya V. Zapolskih, Nikita A. Kovalenko, Irina A. Uspenskaya
- P36** *Phase equilibria in the Na⁺ - K⁺ - HCO₃⁻ - CO₃²⁻ - NO₃⁻ - H₂O - CO₂ system at 25 and 50°C*
Ekaterina V. Belova, Svetlana V. Kurdakova, Mikhail N. Mamontov, Nikita A. Kovalenko, Irina A. Uspenskaya
- P37** *Thermodynamic modeling of the neodymium and samarium nitrates separation by the TBP extraction*
Aleksey I. Maksimov, Nikita A. Kovalenko
- P38** *Thermodynamic Properties of Mixed Solutions of Rare Earths and Calcium Nitrates*
Alexander V. Dzuban, Alexander V. Nesterov
- P39** *Solubility and diffusion of small molecules in polyethylene composites*
Martin Bohln, Edvin Erdtman, **Peter Ahlström**, Mikael Berlin, Thorbjörn Andersson, Thomas Gkourmpis, Kim Bolton
- P40** *Viscosities of 1-alkyl-3-methylimidazolium ionic liquids and their binary mixtures with acetonitrile*
Oana Ciocîrlan, Olga Iulian
- P41** *Evaluation of thermodynamic properties of solketal esters for applications as fuel additives*
Diana Adela Berinde, Giorgiana Dana Barbu, Valentin Plesu, Petrica Iancu, Adrian Victor Crisciu, Nicoleta Gabriela Stefan



29th European Symposium on Applied Thermodynamics – ESAT 2017
May 18-21, 2017, Radisson Blu Hotel, Bucharest, ROMANIA

Poster Program

Molecular & statistical thermodynamics

- P42 *Thermodynamics of supercooled steam: Molecular simulation results and theory*
Filip Moučka, **Ivo Nezbeda**
- P43 *Impact of the equation of state on calculated adsorption isotherm using DFT*
Julian Butz, Patrick Zimmermann, Sabine Enders
- P44 *Molecular Simulation of Crown-Ethers*
Seyed Hossein Jamali, Mahinder Ramdin, Shwet Kumar Rinwa, Wim Buijs, Thijs J. H. Vlugt
- P45 *Development and Implementation of Efficient Continuous Fractional Component Monte Carlo Algorithms*
Ali Poursaeidesfahani, Ahmadreza Rahbari, Ariana Torres-Knoop, Remco Hens, David Dubbeldam, Thijs J. H. Vlugt
- P46 *Parametrization of PC-SAFT using experimental results for surface tension and molecular simulation results for enthalpies of evaporation*
Jonas Mairhofer, Joachim Gross
- P47 *Thermodynamics of Self-Assembly of Perylene Derivatives*
Jörg Baz and Niels Hansen
- P48 *Computational Based Material Property Prediction of NH₃/IL Working Pairs for Absorption Refrigeration Cycles*
Tim M. Becker, Meng Wang, Abhishek Kabra, Carlos A. Infante Ferreira and Thijs J.H. Vlugt
- P49 *Evaluation of a New Combination Rule to Predict Adsorption of n-Alkanes in Silicalite*
Maria Gabriela M V Pereira, Sarah Arvelos, Thalles S Diógenes, **Lucienne L. Romanielo**
- P50 *Quantum mechanical calculations on azulene ligands for complexing chemically modified electrodes*
Maria-Daniela Pop, Amalia Stefaniu, Gabriela Stanciu, Liviu Birzan, Lucia Pintilie, **Eleonora-Mihaela Ungureanu**



29th European Symposium on Applied Thermodynamics – ESAT 2017
May 18-21, 2017, Radisson Blu Hotel, Bucharest, ROMANIA

Poster Program

Alternative solvents, Supercritical fluids

- P51 *Extraction of Salvia fruticosa with supercritical CO₂: Mathematical modelling and comparison with other extraction methods*
Daphne Kavoura, Konstantina Kyriakopoulou, Georgios Papaefstathiou, Vasiliki Louli, Konstantinos Gardikis, Nektarios Aligiannis, Magdalini Krokida, **Epaminondas Voutsas**, Kostis Magoulas
- P52 *Challenges in the Development of Deep Eutectic Solvents*
Catarina Florindo, Luis C. Branco, **Isabel M. Marrucho**
- P53 *Influence of the α -function and critical parameters prediction method on the quality of solid-supercritical fluid equilibrium representation*
Mihaela Popescu, Petrica Iancu, Adrian V. Crisciu, Valentin Plesu

Carbon capture & storage, Renewable energy/Alternative energy resources & storage

- P54 *A short-cut method for assessing solvents for gas cleaning by reactive absorption*
Dan Vasiliu, Erik von Harbou, Hans Hasse
- P55 *Viscosity and density measurements of aqueous amines at high pressures*
Eduardo I. Concepción, Jorge Rubio, **Rodrigo Susial**, Miguel A. Villamañán, M. Carmen Martín
- P56 *SiModEx: a combination of reactive molecular Simulation, thermodynamic Modelling and Experiments for CO₂ capture processes understanding*
Yohann Coulier, Elena Baboi, Florent Goujon, Jean-Yves Coxam, Braden Kelly, Weikai Qi, William R. Smith, **Karine Ballerat-Busserolles**
- P57 *Q-electrolattice equation of state: application to pressure retarded osmosis*
Fahim Bin Abdur Rahman, Marcelo Castier, Ahmed Abdel-Wahab
- P58 *Impact of equation of state on supercritical CO₂ Brayton cycle process design*
Qiao Zhao, Mounir Mecheri, Thibaut Neveux, Romain Privat, **Jean-Noël Jaubert**



29th European Symposium on Applied Thermodynamics – ESAT 2017
May 18-21, 2017, Radisson Blu Hotel, Bucharest, ROMANIA

Poster Program

Colloids, surfactants & interfacial phenomena

- P59 *Enhanced Oil Recovery using Ionic Liquids Blends: Phase Behavior*
Iria Rodríguez-Escontrela, Raquel Corchero, Maura Puerto, Clarence Miller, George Hirasaki and **Ana Soto**
- P60 *Equilibrium and Nonequilibrium Thermodynamics of Planar and Curved Interfaces*
Øivind Wilhelmsen, Thuat T. Trinh, Anders Lervik, Elisa Magnanelli, David Reguera, Signe Kjelstup, Dick Bedeaux

Gas & oil (downstream and upstream), petrochemicals, hydrofracking

- P61 *Shortcut modeling of supersonic gas separators*
Marcelo Castier
- P62 *Phase equilibria of mercury in natural gas using UMR-PRU model*
Vassilis Koulocheris, Vasiliki Louli, **Epaminondas Voutsas**
- P63 *Phase Equilibrium Modeling for the DME Enhanced Water-flooding*
Christos Tsanas, Erling H. Stenby, Wei Yan
- P64 *Prediction of Dew Point and Liquid Dropout of Natural Gas and Gas Condensates*
Nefeli Novak, Eirini Petropoulou, Anthi Plakia, Constantinos Pittas, Vasiliki Louli, Georgia Pappa, Christos Boukouvalas, Epaminondas Voutsas
- P65 *Simulation of a Natural Gas Dehydration Process with the UMR-PRU model*
Eirini Petropoulou, Georgia D. Pappa, Kostis Magoulas, **Epaminondas Voutsas**
- P66 *Modeling and Simulation of Oil Refining Processes*
Ancuta Alexandra Neagu, Valentin Plesu, Gheorghe Bumbac, Petrica Iancu



29th European Symposium on Applied Thermodynamics – ESAT 2017
May 18-21, 2017, Radisson Blu Hotel, Bucharest, ROMANIA

Poster Program

Materials (polymers, metals, inorganic solids, liquid crystals), Nanoscience & nanotechnology

- P67 *Polyazulene based materials for heavy metal ions detection*
Valentin Stanescu, Cecilia Iordache, Ionut Stanescu, Magdalena-Rodica Bujduveanu, Veronica Anastasoae, Maria-Daniela Pop, **Eleonora-Mihaela Ungureanu**
- P68 *Thermodynamic study on the complexation of molybdenum (VI) with D-(-)-quinic acid in water + methanol solutions by LFE equation*
Kavosh Majlesi, Mehrdokht Fahmi
- P69 *Functionalization of graphene materials through aryl diazonium chemistry - an approach for amperometric biosensors with higher sensitivity and selectivity*
Matei Raicopol, **Luisa Pilan**
- P70 *Thermodynamic stability of bovine plasma fibrinogen in the presence of nanoparticles*
Daniela Gheorghe, Aurica Precupaş, Alina Botea-Petcu, Vlad Tudor Popa, **Speranța Tănăsescu**
- P71 *Thermodynamic study of protein stability in the presence of SiO₂ nanoparticles*
Alina Botea-Petcu, Aurica Precupaş, Daniela Gheorghe, Romică Sandu, Vlad Tudor Popa, **Speranța Tănăsescu**

Pharmaceuticals & cosmetics

- P72 *Influence of polymers on the aqueous solubility of pharmaceuticals*
Clarissa Lechtenberg, Lisa Vahle, Marius Berndt, Markus Thommes, Gabriele Sadowski
- P73 *Thermophysical characterization of mixtures of montmorillonite with water of different mineralization for uses in pelotherapy*
Jesús Rosino, Carmen P. Gómez, **Marta M. Mato**, M. Lourdes Mourelle, José L. Legido

Teaching Thermodynamics

- P74 *Emphasizing Connections between Real-Gas Mixtures, Gas Ideal-Solutions, and Perfect-Gas Mixtures*
Romain Privat, Jean-Noël Jaubert, **Edouard Moine**



29th European Symposium on Applied Thermodynamics – ESAT 2017
May 18-21, 2017, Radisson Blu Hotel, Bucharest, ROMANIA

Poster Program

Novel reaction & separation technologies (e.g., ionic liquids, electrolyte systems, membranes, gas hydrates)

- P75 *Separation of ethylbenzene/styrene compounds in ternary LLE with ionic liquids*
Urszula Domańska-Żelazna, Michał Wlazło, Monika Karpińska
- P76 *Separation of hex-1-ene/hexane and cyclohexene/cyclohexane with ionic liquids*
Urszula Domańska-Żelazna, Michał Wlazło, Monika Karpińska
- P77 *Desulfurization: cross-solubility between deep eutectic solvents or ionic liquids and fuel oil*
Filipa Lima, Armando Silvestre, Luís Branco, **Isabel Marrucho**
- P78 *Liquid–liquid extraction of sulfur compounds from model fuels using tricyanomethanide based ionic liquids or DES*
Marek Królikowski
- P79 *Comprehensive Evaluation of COSMO-RS Approach Performance in Predicting Infinite Dilution Activity Coefficients of Molecular Compounds in Ionic Liquids*
Kamil Paduszyński
- P80 *Purification of biomolecules using PEG and biodegradable salts*
Kamila Wysoczanska, Eugénia A. Macedo
- P81 *Influence of Polymer Concentration on Membrane Performance in Wastewater Treatment*
Laurenția Geanina Tiron, Ștefan Cătălin Pintilie, Andreea Liliana Lazăr, Maria Vlad, Ștefan Baltă, Marius Bodor
- P82 *Influence of ZnO nanoparticle size on the performance of polysulfone membranes*
Ștefan Cătălin Pintilie, **Laurenția Geanina Tiron**, Andreea Liliana Lazăr, Cristian Eni, Iulian Gabriel Bîrsan, Ștefan Baltă



29th European Symposium on Applied Thermodynamics – ESAT 2017
May 18-21, 2017, Radisson Blu Hotel, Bucharest, ROMANIA

Poster Program

Product & process design

- P83 *Modeling of the spray process in the natural gas transport tank*
Xiaochun Xu, Ibrahima Noba, Romain Privat, Jean-Noël Jaubert
- P84 *Revision and Extension of Group Contribution Methods for Predicting Physical Properties of Pure Ionic Liquids*
Kamil Paduszyński
- P85 *SPEED Lipids Database for Process-Product Design*
Olivia A. Perederic, Sawitree Kalakul, Bent Sarup, John M. Woodley, Rafiqul Gani
- P86 *Sensitivity of Process Design to Phase Equilibrium Uncertainty: Comparative Study*
Leon Burger, **Cara E. Schwarz**
- P87 *PVC Flooring Recycling with the Selective Dissolution/Precipitation Technique*
Andreas Paraskeva, Andia Christou, **Eleni Boli**, Alain Casoli, Dominique Robert, Feliks Bezati, Georgia Pappa, Kostis Magoulas
- P88 *Fixed bed catalytic reactor modelling for TAME synthesis*
Valentin Plesu, Alexandra-Elena Bonet-Ruiz, Petrica Iancu, Jordi Bonet, Enric Botella, Stefan Toader, Nicoleta Gabriela Stefan
-