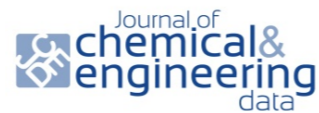# 31st European Symposium on Applied Thermodynamics

Abstract Book

This abstract book has been based on the program as of 25 June 2021

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Click on each conference title to go to the abstract

Central European Summer Time

Monday 5 July

Time			
9:00	Welcome period		
10:30	Welcome address		
Chair:	COQUELET Christophe - Mines ParisTech		
11:00	**Keynote Speaker - François Nicol, Veolia Research** (available in replay) Process industry of the future: SFGP vision		
11:45	Ice breaker		
12:15	Break		
13:45	SADOWSKI Gabriele - TU Dortmund University		
	Keynote Speaker - Antoon Ten Kate, Nouryon (available in replay) Electrolytes in industry: worth their salt		

	Session 1A	Session 1B - IUT	Session 1C
Chairs:	WILHELMSEN Oivind - Norwegian University of Science and Technology	PASSARELLO Jean-Philippe - LSPM - CNRS UPR 3407	JAUBERT Jean-Noel - LRGP CNRS
	MS applied	**Electrolytes - Applications**	**Models**
14:35	**15 - A. Rahbari**, Delft Univ. of Technology Solubility of water in hydrogen at high pressures: A molecular simulation study	**133 - M. Williams-Wynn**, Univ. of KwaZulu-Natal, South Africa The distribution coefficients of Nd3+ between HNO3 and HDEHP	**18 - S. Hirohama**, Aveva, United-Kingdom Test of Inclusive gE Formula for Holderbaum-Gmehling Mixing Rule (PSRK) to Use NRTL together with Quadratic Mixing Rule with Temperature Dependent kji
14:55	**97 - E. Bourasseau**, CEA, France Thermodynamic properties study of MOX nuclear fuel using molecular simulation methods	**286 - D. Abranches**, Univ. of Aveiro, Portugal The Impact of the Counterion in the Performance of Ionic Hydrotropes	**23 - R. Privat**, Univ. of Lorraine, France New insight on EoS/gE mixing rules for cubic equations of state: proposition of a unified approach
15:15	**115 - P. Petris**, Siemens Industry Software B.V., The Netherlands From COSMO to advanced molecular simulations	**333 - C. Pulido Lamas**, Univ. Compluetense of Madrid, Spain Freezing point depression for salty water using a scaled charge model	**219 - E. Moine**, Prosim, France Application of a comprehensive methodology for benchmarking a thermodynamic model
15:35	Break - The exhibitors welcome you on their booth		

	Session 2A	Session 2B - IUT	Session 2C
Chairs:	BOURASSEAU Emeric - CEA	SIMONIN Jean-Pierre - Sorbonne Université CNRS	MEJIA Andres - Universidad de Concepcion
	Mesophases	**Electrolytes - Theory**	**Models**
15:55	**154 - A. Galindo**, Imperial College, United-Kingdom Self-assembly of the mesophases of aqueous monoglycerides using coarse-grained SAFT force fields	**139 - L. André**, BRGM, France Thermodynamics of saline aqueous solutions	**239 - D. Qvistgaard**, Technical Univ. of Denmark New Association Schemes for Tri-Ethylene Glycol (TEG)
16:15	**50 - G. Perez-Sanchez**, Ciceco, Portugal Unravelling the Phase Behaviour of Imidazolium-based Ionic Liquid Aqueous Solutions through Coarse-Grain Molecular Dynamics Simulations	**350. A. Gonzales de Castilla**, Institute of Thermal Separation Processes, Germany : A modified closest approach parameter for the Pitzer-Debye-Hückel term to address underscreening in 1:1 electrolytes with low dielectric constants	**282 - J. N. Jaubert**, Univ. of Lorraine, France Search for the optimum values of the (u,w) parameters involved in cubic equation of state - discussion on the impact of a volume translation
16:35	**337 A. Victorov**, Saint Petersburg State Univ., Russia Specific interactions in the model of mixed nonionic micelles: predicting aggregation behavior and details of structure	**141 - X. Liang**, Technical Univ. of Denmark On the parameters used in the Debye-Hückel theory	**324 - C. S. Agger**, Calsep, Denmark Modified method of characteristics for generating EOR oil recovery curves
16:55	Break - The exhibitors welcome you on their booth		
17:05	**Student activity: Meet your hero** **The exhibitors welcome you on their booth**		

Tuesday 6 July

Time			
	announce		
9:00	Welcome period		
Chair:	GALINDO Amparo - Imperial College London		
9:30	**Keynote Speaker - Joachim Gross, Univ. Stuttgart** (available in replay) A new approach for constructing analytic equations of state Sponsored by Entropy		
Chair:	MACEDO Maria Eugénia - University of Porto - FEUP		
10:15	**3 min pitches for Helmut Knapp best poster awards - sponsored by CNRS**		
10:55	Break - The exhibitors welcome you on their booth		

	Session 3A	Session 3B - IUT	Session 3C
Chairs:	LLOVELL Felix - Universitat Rovira i Virgili	HASLAM Andrew - Imperial College London	BLAS Felipe - Universidad de Huelva
	Interfaces	**Electrolyte - Industry**	**SAFT**
11:10	**64 - S. Stephan**, Lab. of Engineering Thermodynamics, Germany Enrichment of components at vapor-liquid interfaces: molecular modeling and prediction from macroscopic data	**91 - B. Maribo-Mogensen**, Hafnium Labs, Denmark To infinite dilution and beyond – perspectives on predictive electrolyte models	**14 - B. D. Marshal**, Exxon Mobil A doubly associated reference perturbation theory for water
11:30	**122 - A. Mejia**, Univ. de Concepcion, Spain Experimental determination, theoretical modeling and molecular dynamics simulation of interfacial properties of CH4 + n-alkane binary mixtures	**352 - A. Bansal**, Aveva, USA Process modeling of electrolyte systems using equation-oriented framework in AVEVA™ Process Simulation	**32 - K. Langenbach**, Lab. of Engineering Thermodynamics, Germany Thermodynamic and dielectric properties from an equation of state
11:50	**132 - S. Tiwari**, Indian Institute of Technology, Kampur, India Insight into the mechanism of nanoparticle induced suppression of detergency: experiments, modelling and simulations	**260 - S. Kuitunen**, Neste Neste's view on needs for electrolyte thermodynamics	**54 - L. F. Vega**, Khalifa Univ. of Abu-Dhabi, U.A.E Extension of soft-SAFT EoS to polar fluids: Comparison with molecular simulations and application to experimental systems
12:10	**POSTER SESSION 1** **The exhibitors welcome you on their booth**		

	Session 4A	Session 4B	Session 4C
Chairs:	NIETO-DRAGHI Carlos - IFP Energies nouvelles	TEN KATE Antoon - Nouryon	GROSS Joachim - University of Stuttgart
	IFT / confinement	**IUT**	**SAFT**
14:10	**89 - R. Nagl**, Graz Univ. of technology, Austria Interfacial Properties in ternary and quaternary Systems		**120 - T. van Westen**, Univ. of Stuttgart, Germany Accurate first-order perturbation theory for fluids: uf-Theory
14:30	**51 - I. Polishuk**, Israel About interrelation between PVT and phase equilibria in the systems of Ionic Liquids		**128 - J. T. Cripwell**, Stellenbosch Univ. Dipolar SAFT-γ Mie: extension to secondary groups and isomers
14:50	**164 - A. Mio**, Univ. of Trieste, Italy Investigation of friction force trends at the nanoscale using computation approach		**71 - M. Kohns**, Imperial College, United-Kingdom Modelling aqueous solutions of strong and weak electrolytes using the SAFT-γ Mie equation of state
15:10	Break The exhibitors welcome you on their booth	**Round table discussion on Industrial Use of Electrolyte Thermodynamics.** The debate will cover 3 questions: 1. What modeling approach do you use when confronted with an electrolyte problem? 2. How to parameterize a model in the absence of data 3. How to create collaboration on an industrially important issue	Break The exhibitors welcome you on their booth

	Session 5A		Session 5C
Chairs:	MOULTOS Othon - TU Delft		MCCABE Clare - Vanderbilt University
	Confined fluids		**SAFT**
15:25	**295 - H. Adidharma**, Univ. of Wyoming, U.S.A. New isochoric method to measure the phase transitions of binary mixtures confined in nanopores		**112 - M. Kiesel**, Imperial College of London Structural Properties of Ionic Surfactants using a SAFT-γ Mie Force Field in Molecular Simulation
15:45	**70 - I. G. Economou**, Institut of Nanoscience & Nanotechnology, Greece Mesoscale Modelling of Fischer-Tropsch Product Mixtures Confined in Graphene Meso-Pores		**364 - P. Rehner**, Univ. of Stuttgart, Germany A model for non-ionic surfactants based on inhomogeneous PC-SAFT
16:05	**322 - P. Habibi**, Delft Univ. of technology, The Netherlands A DFT study of the hydrogen storage capabilities of 2D honeycomb borophene oxide		**309 - E. J. M. Filipe**, Univ. of Lisboa, Portugal Complete surface tension characterization of fluorinated alcohols and their mixtures with hydrogenated alcohols: experimental, soft-SAFT-DGT modeling and MD simulations
16:25	**Job forum** **The exhibitors welcome you on their booth**		

PREDICTION OF PHASE DIAGRAMS AND PH-SOLUBILITY PROFILES OF ACTIVE PHARMACEUTICAL INGREDIENTS USING THE SAFT-γ MIE GROUP CONTRIBUTION APPROACH

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The pharmaceutical industry is facing a constantly rising demand for drugs of growing complexity and more efficient manufacturing processes. The solubility of pharmaceuticals is a key property during the drug formulation and the subsequent design of the processes involved in the manufacturing of the drug. Common challenges in these manufacturing processes include: the large number of experiments required and the extremely low solubilities of active pharmaceutical ingredients (APIs) in water for which experiments are difficult to perform. Computer-aided approaches provide an attractive alternative to performing time-consuming and costly experiments. Specifically, molecular modelling approaches can deliver physical properties predictively, including phase equilibria and solubility.

The SAFT-γ Mie group contribution (GC) equation of state (EoS) [1, 2] is such a predictive thermodynamic modelling technique. In the SAFT-γ Mie framework, molecules are modelled as heteronuclear chains formed from fused spherical segments, which represent the distinct functional groups comprising the molecule. In this framework, it is assumed that the properties of a molecule or a mixture can be determined from the weighted contributions of the functional groups present in the system of interest, with the assumption that the parameters characterizing the functional groups are fully transferable across molecules.

We first demonstrate the validity of the SAFT-γ Mie EoS in the prediction of thermodynamic equilibrium properties of neutral APIs including solubilities. We then develop the complete phase diagrams of the APIs in water which clearly outline the solid-liquid, liquid-liquid and vapour-liquid equilibria for these mixtures. Moreover, as it is well known that the bioavailability of a drug is improved by salt formulation, we test our approach for the solubility prediction of ionisable APIs, and their salts, under changing pH. The SAFT-γ Mie EoS accounts for the complex speciation phenomena that take place under pH changes including fully ionised (strong electrolytes) and partially ionised (weak electrolytes) systems. We investigate in particular, the solubility of the acidic APIs, ibuprofen and ketoprofen, their speciation and salt formation, to develop the pH-solubility profiles for these drugs. We also study the effect of various counter-ions on the pH-solubility profiles of these APIs and their salts.

[1] Papaioannou, V. *et al.* Group contribution methodology based on the statistical associating fluid theory for heteronuclear molecules formed from Mie segments. *Chem. Phys.* 140, (2014).

[2] Dufal, S. *et al.* Prediction of thermodynamic properties and phase behavior of fluids and mixtures with the SAFT-γ mie group-contribution equation of state. *J. Chem. Eng. Data* 59, 3272–3288 (2014).

ePC-SAFT MODELING OF L-TRYPTOPHAN PARTITIONING IN AQUEOUS BIPHASIC SYSTEMS WITH AMINO ACID ALKYLIMIDAZOLIUM IONIC LIQUIDS

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Aqueous biphasic systems (ABSs) containing alkylimidazolium ionic liquids (ILs) and inorganic salts are considered as promising media for the extraction of biomolecules, e.g., amino acids. Molecular design of ILs helps to find the ABSs with the desired extraction capacity, which is one of the major aspects of their practical application. In view of the ever-increasing amount of new ILs, it becomes particularly important to predict phase behaviour and partitioning of target solutes in IL-based ABSs. Amino acid ILs (AAILs) attract special attention because of their biodegradability and low toxicity [1].

In this work we apply ePC-SAFT (Electrolyte Perturbed-Chain Statistical Associating Fluid Theory) for modelling liquid-liquid equilibria and the distribution of L-tryptophan between the liquid phases in aqueous solutions of 1-butyl-3-methylimidazolium AAILs (containing anions of L-Leucine, L-Valine or L-Lysine) with added salt (K_3PO_4). New parameters of the model have been estimated from our experimental data on liquid-liquid equilibrium. All calculation procedures were implemented using the Fortran Power Station 4.0 software package. For all AAILs systems studied in this work, calculated liquid-liquid equilibrium and partitioning of L-tryptophan between the liquid phases is in satisfactory agreement with experiment, demonstrating that ePC-SAFT equation of state is a useful tool for modeling liquid-liquid equilibrium and the extraction capacity of the AAILs-based ABSs.

Acknowledgements

References

[1] Egorova, K. S., Seitkalieva, M. M., Posvyatenko, A. V., & Ananikov, V. P. (2014). An unexpected increase of toxicity of amino acid-containing ionic liquids. Toxicology Research, 4(1), 152-159.

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