France – 100% Virtual – 5-9 July 2021

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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Normal sessions
IUT sessions on electrolyte thermodynamics
SAFT Symposium sessions

Click on each conference title to go to the abstract

Central European Summer Time

Monday 5 July

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		
	SADOWSKI Gabriele - TU Dortmund University		
13:45	**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. Complutense 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

	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 macrosopic 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	**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	**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		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**		

SPECIFIC INTERACTIONS IN THE MODEL OF MIXED NONIONIC MICELLES: PREDICTING AGGREGATION BEHAVIOR AND DETAILS OF STRUCTURE

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Modeling aggregation in solutions of mixed surfactants is an important task that has been attracting attention for years. Classical molecular-thermodynamic micellization models [1] do not explicitly take into account the specific interactions that may occur between complex polar heads of many nonionic surfactants, neither the hydration water within the coronae of mixed micelles. Such specific interactions have been described in our previous model of the standard free energy of aggregation [2], using the quasichemical GE model that is applied locally in the corona of the spherical micelles. In this work, we extend our previous model by including wormlike aggregates and by describing the aggregation equilibrium and shape transitions in solutions of varying total concentration of surfactants. We apply the model to predict the aggregation behaviour of aqueous mixtures of Triton X-114 (nonionic ethoxylated surfactant) with added 1-octanol and demonstrate its fair performance by comparing both with our own experiment and literature data. In our experiment, we determine the partition coefficient of 1-octanol between the micelle and the aqueous environment from the headspace analysis data; we also measure the critical micelle concentration (CMC), and aggregation numbers.

Apart from the aggregation characteristics that are usually obtained from the classical aggregation models (CMC, composition, shape and size distribution of the aggregates) our model makes possible to suggest the likely structural details of an aggregate. Performing calculations for different relative arrangements of the surfactant and octanol molecules within the aggregate, the model serves to establish the optimal structure of the aggregate and answer (within its approximations) a number of important questions, e.g., how deep the octanol molecules penetrate in the micellar core, how strong is the hydration of the corona, what is the number of hydrogen bonds in it, etc.

Acknowledgment

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References

[1] Self -Assembly: From Surfactants to Nanoparticles, Ed. R. Nagarajan, 2019. Wiley & Sons.

[2] A.I. Victorov, Modeling of Micelle-Solution Equilibria for Mixed Nonionic Micelles with Strong Specific Interactions in Coronae: Group-Contribution Approach. J. Chem. Eng. Data 59 (2014) 2995−3002.

The distribution coefficients of Nd^{3+} between HNO_3 and HDEHP

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Abstract

For the true implementation of the circular economy,[1] there is a need for the development of recycling processes capable of extracting critical materials from waste for reuse. Rare earth metals are some of the critical materials that are used in many high-tech electronic devices.[2] There are presently very few chemical processes available to extract and upgrade these metals to the purities that are required for the manufacture of new electronic devices. To enable the development of chemical processes such as liquid-liquid extraction for the purification processes, an understanding of the phase equilibria and distribution coefficients of the rare earth metals between aqueous and organic phases is required.

Previous studies investigated the distribution of yttrium and europium between an organic and an aqueous phase.[3] In this study, the distribution coefficients of Nd^{3+} ions were measured between an organic phase and an aqueous phase, at differing concentrations of the acid in the aqueous phase at 298 K. The organic phase for these measurements consisted of di-(2-ethylhexyl) phosphoric acid (HDEHP) in a diluent of either n-nonane or n-dodecane, with various concentrations of HDEHP investigated. The aqueous phase consisted of nitric acid. The distribution measurements were conducted in a series of stirred liquid-liquid equilibrium cells. The concentrations of the Nd^{3+} were determined with an ICP-OES.

The measured data were used to optimize a neodymium recycling and purification process which used a counter-current vibrating plate, liquid-liquid extraction column to extract neodymium from a leach liquor and upgrade it to high purities.

References:

1. Geissdoerfer M., Savaget P., Bocken N.M.P., Hultink E.J. (2017). The Circular Economy – A new sustainability paradigm?, J. Clean. Prod. 143, 757-768
2. Tanaka M., Oki T., Koyama K., Narita H., Oishi T. (2013). Chapter 255 - Recycling of Rare Earths from Scrap, Handbook on the Physics and Chemistry of Rare Earths 43, pp. 159-211
3. Williams-Wynn M.D., Naidoo P., Ramjugernath D. (2020). The distribution coefficients of Y^{3+} and Eu^{3+} between HNO_3 and HDEHP. Miner. Eng. [under review].

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