



Normal sessions - Auditorium A

IUT sessions on electrolyte thermodynamics - Auditorium B

SAFT Symposium sessions - Auditorium C

Central European Summer Time

Monday 5 July

9:00	Welcome period		
10:30	Welcome address 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		
Ch	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
	WILHELMSEN Oivind - Norwegian University of Science and Technology	BERNARD Olivier - CNRS	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 Nd ³⁺ between HNO ₃ 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 kij
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
	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

9:00	Welcome period 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		
	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
	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	71 - M. Kohns , Imperial College, United-Kingdom Modelling aqueous solutions of strong and weak electrolytes using the SAFT-γ Mie equation of state

11:30	122 - A. Mejia , Univ. de Concepcion, Spain Experimental determination, theoretical modeling and molecular dynamics simulation of interfacial properties of CH ₄ + n-alkane binary mixtures	260 - S. Kuitunen , Neste Neste's view on needs for electrolyte thermodynamics	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	372 - P. J. Walker , Imperial College of London Importance of the relative static permittivity in electrolytic SAFT-VR Mie equations of state	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
	NIETO-DRAGHI Carlos - IFP Energies nouvelles IFT / confinement	TEN KATE Antoon - Nouryon IUT	GROSS Joachim - University of Stuttgart 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		14 - B. D. Marshal , Exxon Mobil A doubly associated reference perturbation theory for water
15:10	Break The exhibitors welcome you on their booth Session 5A		Break The exhibitors welcome you on their booth Session 5C
	MOULTOS Othon - TU Delft Confined fluids		MCCABE Clare - Vanderbilt University 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		

Wednesday 7 July

9:00	Welcome Period DE HEMPTINNE Jean-Charles - IFP Energies nouvelles		
10:00	EFCE Michael Michelsen award lecture 2020 - Gabriele Sadowski, TU Dortmund (available in replay) Thermodynamics for Pharmaceutical Development Sponsored by Elsevier		
10:45	Break - The exhibitors welcome you on their booth		
10:55	MOUGIN Pascal - IFP Energies nouvelles Session 6A	DUSSAP Claude-Gilles - Institut Pascal Session 6B	FILIFE Eduardo - Instituto Superior Técnico Session 6C
	Molecular design	Electrolyte - Theory	SAFT
11:10	165 - M. Fermeglia , Univ. of Trieste, Italy How molecular simulations can inform business decisions in different industrial sectors: the compositelator example	49 - O. Bernard , CNRS, France Thermodynamic properties of polyelectrolytes and associating electrolytes in solution	99 - M. Fischschweiger , Graz Univ. of technology, Austria Modeling of Diffusion in Highly-Crosslinked Epoxy Resins with Maxwell-Stefan Approach and PC-SAFT
11:30	327 - T. Specht , Lab. of Engineering Thermodynamics, Germany Quantitative fingerprinting and thermodynamic modeling of poorly specified mixtures with NMR spectroscopy and machine learning	370 - S. Hassanjani Saravi , Princeton Univ. U.S.A. Activity coefficients and relative permittivity of aqueous electrolytes from molecular simulations	114 - J. Eller , Univ. of Stuttgart, Germany Adsorption in heterogeneous porous media using classical density functional theory based on the PC-SAFT equation of state
11:50	271 - M. Popovic , Techn. Univ. of Munich, Germany Thermodynamic characterization of viruses: enthalpy, entropy and Gibbs energy	323 - J.P. Simonin , CNRS, France About the "Born" term used in thermodynamic models for electrolytes	170 - A.Reinhardt , KIT, Germany Interfacial properties of water + long-chain molecules
12:10	POSTER SESSION 2 The exhibitors welcome you on their booth		
	Session 7A	Session 7B	Session 7C
	BRENNECKE Joan - University of Texas at Austin Molecular design	MARIBO-MOGENSEN Bjorn - Hafnium Labs Electrolyte EOS	PARICAUD Patrice - ENSTA PARIS SAFT
14:10	19 - J. Ilja Siepmann , Univ. of Minnesota, U.S.A. High-Throughput Simulations and Machine Learning for Adsorption in Nanoporous Materials: Applications to Storage and Separations	352 - A. Bansal , Aveva, USA Process modeling of electrolyte systems using equation-oriented framework in AVEVA™ Process Simulation	113 - C. G. Alba , Univ. of Ramon Llull, Spain Study of the Solubility of 4th Generation Refrigerant R513a with Compatible Lubricants and their Performance in Refrigeration Cycles using Polar Soft-SAFT
14:30	301 - C. Mc Cabe , Vanderbilt Univ. of Nashville, USA Utilizing the Molecular Simulation Design Framework (MoSDeF) to Screen Soft Matter Systems	291 - S. Kournopoulos , Imperial College of London SAFT- γ Mie models for aqueous organic electrolytes: simulation benchmarks and development of a model for carboxylate salts	213 - F. Llovel , Univ. of Ramon Llull, Spain Characterization of the Absorption of F-Gases in new Fluorinated Ionic Liquids and Deep Eutectic Solvents with Soft-SAFT
14:50	234 - Silvana Mattedi e Silva - U. Federal de Bahia, Salvador, Brazil Improvement of artemisinin solubility using ionic liquids as hydrotropes	345 - L. Cassayre , CNRS, France A thermodynamic model representing solid-liquid equilibria in the VOSO ₄ -H ₂ SO ₄ -H ₂ O system based on water activity and solubility measurements	248 - F. J. Blas , Univ. de Huelva, Spain Interfacial properties of coarse-grained models of greenhouse gases, refrigerants, and long alkanes from density functional theory and computer simulation
15:10	Break - The exhibitors welcome you on their booth		



	Session 8A	Session 8B	Session 8C
	FERMEGLIA Maurizio - University of Trieste	CASSAYRE Laurent - Laboratoire de Génie Chimique/Toulouse INP	CHAPMAN Walter - Rice University
	Molecular design	Electrolytes - Molecular Simulation	SAFT
15:30	37 - F. Jirasek , Univ. of California, Irvine, USA Prediction of Activity Coefficients with Machine Learning	204 - C. Nieto-Draghi , IFPEN, France Coarse-graining simulation of the thermodynamic and mechanical behaviour of semi-permeable membranes used in redox flow batteries	40 - O. Wilmhelsen , Norwegian Univ. of Science & Technology SAFT for quantum fluid mixtures and the hydrogen society: present state-of-the-art and fundamental challenges
15:50	134 - A. Alhadid , Technical Univ. of Munich, Germany Design of Deep Eutectic Solvents: Selecting Constituents Based on Molecular Structure	232 - P. T. Cummings , Vanderbilt Univ. of Nashville, USA Molecular Modeling of Supercapacitors	339 - N. Novak , NCSR, Greece Modeling of water-hydrocarbon phase equilibria with the SAFT-VR Mie equation of state
16:10	355 - P. Krokidas , Nat. Center for Scientific Research, Greece Physics-driven machine learning model for the design of highly selectivity zeolitic-imidazolate frameworks	307 - W. R. Smith , Univ. of Guelph, Canada Molecular Simulation of Reactive Electrolyte Solutions and Applications to CO2 Capture	116 - T. Lafitte , Siemens/PSE, U.K The use of SAFT-γ Mie EoS in industrial process modelling applications
16:30	Job forum The exhibitors welcome you on their booth		

Thursday 8 July

	Session 9A	Session 9B	Session 9C
08:45	EL AHMAR Elise - Mines ParisTech	FELE ZILNIK Ljudmila - National Institute of Chemistry	HELD Christoph - TU Dortmund University
	Experimental	Innovative processes	SAFT
9:40	274 - D. Tuma , Fed. Inst. for Materials Research & Testing, Germany Carbon dioxide solubility in the ionic liquid 1-Hexyl-3-methylimidazolium hexafluorophosphate	194 - A. B. Pereira , Univ. Nova de Lisboa, Portugal Mitigation of the environmental impact of fluorinated gases using key enabling technologies	93 - S. Dohrn , TU Dortmund Univ. lab of thermodynamics, Germany Understanding solvent-induced phase separation during spray drying of pharmaceutical formulations using PC-SAFT
10:00	30 - F. Zaidin , Petronas, Malaysia The solubility of CO ₂ + H ₂ S mixtures in water, NaCl and mixed salts aqueous solution at 373.15 K to 423.15 K and pressure up to 25 MPa. experimental and modelling	388 - R. Dohrn , Bayer A.G, Germany Good reporting practice - essential for all who measure or use experimental data	208 - M. Wehbe , Imperial College of London Prediction of phase diagrams and ph-solubility profiles of active pharmaceutical ingredients using the SAFT-γ Mie group contribution approach
10:20	167 - V. Dumouilla , Roquette, France : Raman spectroscopy to model and characterize physicochemical properties of aqueous solutions of carbohydrates and polyols	181 - G. M. Kontogeorgis , Tech. Univ. of Denmark Industrial Requirements for Thermodynamic and Transport Properties - 2020	300 - P. A. Korchak , St-Petersburg State Univ., Russia ePC-SAFT modeling of l-tryptophan partitioning in aqueous biphasic systems with amino acid alkylimidazolium ionic liquids
10:40	Break - The exhibitors welcome you on their booth		
	DOHRN Ralf - Bayer AG		
	A. Aasen EFCE Junior researcher Excellence award (available in replay) Accurate cubic equation of state for quantum fluid mixtures Sponsored by ProSim 		
11:00	Announcement + Helmut Knapp best poster awards		
11:30	POSTER SESSION 3 The exhibitors welcome you on their booth		
11:40			
	Session 10A	Session 10B	Session 10C
	SIEPMANN Joern Ilja - University of Minnesota	YAN Wei - Technical University of Denmark	VEGA Lourdes - Khalifa University
	Hydrates	Non-equilibrium	SAFT
13:40	160 - Saeideh Babae , Univ. of KwaZulu-Natal, South Africa Gas Hydrate Concentration Measurements on Sucrose Solutions Using a New Pilot Test Rig	118 - V. Gerbaud , Univ. of Toulouse, France Extremal principles in non-equilibrium thermodynamics	7 - C. Held , TU Dortmund Univ. lab. of thermodynamics, Germany Predicting the solubility of electrolytes in water-poor media with ePC-SAFT
14:00	359 - M.A. Marcelino Neto , Federal Univ. of technology, Brazil Experimental study and thermodynamic modelling of carbon dioxide and methane hydrates in the presence of isopropanol	197 - T. Zeiner , Graz Univ. of technology, Austria Computational fluid dynamics of ternary extraction systems	243 - W. G. Chapman , Rice Univ. of Houston, USA Self-assembly and phase behavior of mixed patchy colloids with any bonding site geometry: theory and simulation
14:20		80 - A. Dehlouz , Univ. of Lorraine, France Can we efficiently predict fluid viscosity data by combining an equation of state with the entropy-scaling concept?	157 - A. Siddiqi , Univ. of Bath, UK Water effect in the reverse micellar formation of docusate in cyclohexane. A coarse-grained molecular dynamic approach
14:40	Break - The exhibitors welcome you on their booth		
	Session 11A	Session 11B	Session 11C
	FISCHLSCHWEIGER Michael - Clausthal University of Technology	DE ANGELIS Maria Grazia - U. of Edinburgh; INSTM; University of Bologna	VICTOROV Alexey - St. Petersburg State University
	Hydrates	Diffusion	Models
15:00	121 - A. K. Sum , Colorado School of Mines, USA The Applied Thermodynamics of Water as Gas Hydrates: from Molecules to Phase Equilibria	349 - H. M. Polat , Total, France Predicting the transport properties of acid-gases in aqueous MEA solutions using molecular simulations	374 - T. Zhao , Imperial College of London <i>Ab initio</i> development of generalized Lennard-Jones (Mie) force fields for predictions of thermodynamic properties in advanced molecular-based saft equations of state
15:20	144 - A. Serikkali , Mines St Etienne, France Phase equilibrium for sea/waste water treatment and carbon capture with clathrate hydrates	357 - M. S. Santos , Univ. of Queensland, Australia Finite-size effects on the diffusion coefficients from molecular dynamics simulations in crystal-like structures	143 - S. Müller , Hamburg Univ. of technology, Germany Including additional first-principles information into the COSMO-RS-ES model: a study on the local polarizability
15:40	63 - P. Ahlström , Univ. of Borås, Sweden Predicting crystal structures and gas adsorption in organic clathrates	108 - M. Minelli , Univ. of Bologna, Italy A thermodynamic approach for gas sorption in high free volume at cryogenic temperatures	88 - C. Mayer , Graz Univ. of technology, Austria Excess Gibbs-energy models based on discrete modeling of dice-like molecules
16:00	Break		

16:30

Social event - sponsored by Shell



Friday 9 July

09:00

Welcome Period

KUITUNEN Susanna - Neste

10:00

Keynote Speaker - Kamil Paduszynski, Warsaw Univ. of Technology (available in replay)

Discovering Paths from Chemical Structure to Properties of Ionic Liquids with Empirical Correlations and Thermodynamic Models

10:45

Break - The exhibitors welcome you on their booth

Session 12A

SECUIANU Catinca - University Politehnica of Bucharest

Solvent CO2

11:00

6 - M. Bülow, TU Dortmund Univ., Germany
Solvent blends for an increased solubility of sour gases in amine solutions

11:20

138 - F. de Meyer, Total, France
Prediction of CO₂/H₂S/CH₄ solubility in pure water and MDEA, and in an aqueous MDEA solution, using molecular simulations

11:40

320 - F. Tzirakis, Center for research & technology- hellas, Greece
Assessment of phase change solvents used in CO₂ capture

Session 12B

VLUGT Thijs - TU Delft

BioReactors

11:00

340 - F. A. Sanchez, Univ. Nacional del Sur, Argentina
Phase equilibrium engineering in biorefinery reactive systems: n-alkanol acetylation

11:20

265 - R. I. Canales, Univ. Catolica de Chile
Thermodynamic study of the separation of guaiacol from solvents used in the bio-oil catalytic upgrade to fuels

11:40

188 - E. A. Macedo, Univ. of Porto, Portugal
Ethyl lactate-based ATPS for recovery of flavonoids

Session 12C

KIJEVCANIN Mirjana - Faculty of Technology and Metallurgy, University of Belgrade

Algo

11:00

86 - F. de Azevedo Medeiros, Tech. Univ. of Denmark
RAND-based Geochemical Calculation Algorithms for CO₂ Sequestration

11:20

98 - D. Paterson, Linde Engineering, Germany
Volume based formulation for multiphase envelope calculation

11:40

218 - V. Koulocheris, Nat. Technical Univ. of Athens, Greece
Chemical and phase equilibria of mercury in natural gas with the UMR-PRU model

12:00

POSTER SESSION 4

The exhibitors welcome you on their booth

KONTOGEOORGIS Georgios - Technical University of Denmark

Keynote Speaker - Joann Brennecke, Univ. of Texas (available in replay)

Gas Solubilities in Ionic Liquids - Revisited
Sponsored by Chemical Engineering Journal



14:00

14:45

Session 13A

SOTO Ana - Chemical Engineering Department

Solvent CO2

14:45

137 - D. Bahamon, Khalifa Univ. of Abu Dhabi, UAE
Molecular simulations of degraded products in aqueous amines for CO₂ absorption

15:05

258 - E. Hernandez, Univ. Autonoma de Madrid, Spain
Ionic liquid-based catalysts for effective CO₂ valorization to carbonates

15:25

53 - I. I. Alkhatib, Khalifa Univ. of Abu Dhabi, UAE
An integrated approach using soft-SAFT with process modelling for the efficient screening of hybrid solvents for CO₂ capture

15:45

240 - W. G. Chapman, Rice Univ. of Houston, USA
Understanding CO₂ Enhanced Gas Recovery from Gas Competitive Adsorption in Shale Nanopores using Molecular Density Functional Theory

Session 13B

PEREDA Selva - Planta Piloto de Ingenieria Quimica

solvents & Processes

14:45

169 - A. Roth, Karlsruhe Inst. of technology, Germany
Thermodynamic Properties of Water + Polar Polymer + Salt Mixtures

15:05

192 - E. Boli, Nat. Technical Univ. of Athens, Greece
Extraction of bioactive compounds from olive leaves using alternative solvents: experiments and modelling

15:25

81 - P. Stringari, Mines ParisTech, France & N.G. Ince, AVEVA USA
Toward an optimized design of the LNG production process: Measurement and modeling of the solubility limits of p-xylene in methane and methane + ethane mixtures at low temperature

15:45

183 - M. G. De Angelis, Univ. of Bologna, Italy
Measurement and modelling of sorption of CO₂/CH₄/C₂H₆ mixtures in a glassy polymeric membrane for gas separation

Session 13C

PRIVAT Romain - CNRS LRGP

Energy & Safety

14:45

279 - S. Lasala, Univ. of Lorraine, France
The exploitation of reactive working fluids in a closed thermodynamic cycle. A breakthrough high-energy conversion system

15:05

373 - R. Claveau, CEA, France
Toward a physical description of energetic materials sensitivity

15:25

231 - P. Paricaud, ENSTA ParisTech, France
Using ab initio calculation to predict the thermochemical and safety properties of multicomponent systems

15:45

342 - M. Maury, CEA, France
Comparison of approaches to determine lower flammability limits

16:05

Break - The exhibitors welcome you on their booth

16:25

Beekast results

16:30

Closing remarks