

SCIENTIFIC PROGRAM - EQUIFASE 2015

SUNDAY, 28 June

- 16:00 Registration
19:30 Welcome reception and *Cocktail*

MONDAY, 29 June

- 9:00 **Conference Presentation**
9:10 *In memoriam* Hugo Segura.
Andrés Mejía, Universidad de Concepción, Chile
- Chair:** *Cor Peters, The Petroleum Institute, Abu Dhabi, UAE*
- 9:15 **Inaugural Lecture: “Modelling water in computer simulations”**
Carlos Vega, Complutense University of Madrid, Spain
- 10:00 Oral Presentations.
10:00-10:15 Description of solid-liquid equilibria in complex mixtures involved in the acid processing of aluminosilicate ores.
Teyssier Angélique^{1,2}, *Jean-Michel Schmitt*¹, *Christelle Goutaudier*²
¹AREVA, BG Mines, France
²Laboratoire des Multimateriaux et Interfaces, UMR CNRS 5615, Université Claude Bernard Lyon 1, France
- 10:15-10:30 Improved correlations for viscosity of naphthenic crude oils
Krishnaswamy Rajagopal, *Luciana L. de Pinho Rolemberg de Andrade*
Escola de Química / Universidade Federal do Rio de Janeiro, Brazil
- 10:30-10:45 Solid-liquid equilibrium of CuSO₄-H₂SO₄-seawater system
Francisca Justel, *Yecid Jiménez*, *María Elisa Taboada*
Universidad de Antofagasta, Chile
- 10:45-11:00 Solid-solid-liquid equilibrium of lipidic ternary mixtures
*Guilherme J. Maximo*¹, *Rafael T. Aquino*², *Antonio J. A. Meirelles*¹, *Mariana C. Costa*²
¹School of Food Engineering, University of Campinas, Brazil
²School of Applied Sciences, University of Campinas, Brazil
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- 11:00 Poster Session + *Coffee Break*

Chair: *Selva Pereda, PLAPIQUI, Universidad Nacional del Sur, Argentina*

- 11:30 Oral Presentations
11:30-11:45 High-pressure densities and surface tensions of binary and ternary system containing carbon dioxide + n-alkanes.
Constanza Cumicheo, *Marcela Cartes* and *Andres Mejia*
Departamento de Ingeniería Química, Universidad de Concepción, Chile
- 11:45-12:00 Atmospheric densities and interfacial tensions for 1-alcohol (1-butanol to 1-octanol) + water and ether (MTBE, ETBE, DIPE, TAME and THP) + water demixed mixtures.
Andrés Mejía and *Marcela Cartes*
Departamento de Ingeniería Química, Universidad de Concepción, Chile
- 12:00-12:15 The liquid-liquid equilibrium and the solubility in reacting quaternary system acetic acid – n-butanol – n-butyl acetate – water at 293.15–313.15 K
Maria Toikka, *Artemiy Samarov*, *Pavel Naumkin*
Saint-Petersburg State University, Russia
- 12:15-12:30 Gas hydrate phase behavior in presence of organics and electrolytes
*Khalik M. Sabil*¹, *Cor J. Peters*²
¹Heriot Watt University, Eindhoven University of Technology, The Netherlands
²The Petroleum Institute, Abu Dhabi, UAE
- 12:30-12:45 Comments on the correlation of liquid-vapour and liquid-liquid-vapour equilibrium data
Antonio Marcilla, *Maria del Mar Olaya*, *Juan Antonio Reyes*
Chemical Engineering Department, University of Alicante, Spain

- 12:45-13:00 Liquid-liquid-liquid equilibria in systems with surfactant ionic liquids
Iago Rodríguez-Palmeiro, Iria Rodríguez-Escontrela, Oscar Rodríguez, Alberto Arce and Ana Soto
University of Santiago de Compostela, Spain
- 13:00-13:15 Theoretical pre-selection of ionic liquids for liquid-liquid extraction of Neodymium.
Mariusz Grabda^{1,2}, Sylwia Oleszek^{1,2}, Mrutyunjay Panigrahi¹, Dmytro Kozak¹, Franck Eckert³, Etsuro Shibata¹ and Takashi Nakamura¹.
¹*Institute of Multidisciplinary Research for Advanced Materials (IMRAM) Japan*
²*Institute of Environmental Engineering of the Polish Academy of Sciences, Poland*
³*COSMOlogic GmbH & Co KG, Germany*

13:30

Lunch

Chair: *Marcelo Castier, Texas A&M University at Qatar, Qatar*

- 15:00 Oral Presentations.
- 15:00-15:15 Measurement of CO₂ + freon phase equilibria and extension of the predictive E-PPR78 equation of state to freon-containing systems
Jean-Noël Jaubert¹, Romain Privat¹, Jun-Wei Qian¹, Niramol Juntarachai¹ and Christophe Coquelet²
¹*ENSIC - LRGP - University of Lorraine, France*
²*CTP-Mines Paristech, France*
- 15:15-15:30 Extension of the Soft-SAFT thermodynamic model to derivative and transport properties
Felix Llovel, Lourdes F. Vega
MATGAS 2000 AIE, Spain
- 15:30-15:45 Usability of the semi-predictive NRTL-SAC model for processing and evaluation of phase equilibrium
Karel Reháč, Jiri Velas, Pavel Morávek and Aigerim Mustafina
University of Chemistry and Technology, Prague, The Czech Republic
- 15:45-16:00 Phase behaviour and interfacial properties of CO₂ + n-alkane binary mixtures: Coarse-Grained theoretical modelling and Molecular Simulations
Harry Cárdenas, Andrés Mejía
Departamento de Ingeniería Química, Universidad de Concepción, Chile
- 16:00-16:15 Phase stability analysis in the vicinity of singularities
Dan Vladimir Nichita
CNRS UMR 5150, Laboratoire des Fluides Complexes et leurs Reservoirs/Université de Pau et des Pays de l'Adour, France
- 16:15 **Esteban A. Brignole Award**
Presentation: Marcelo Castier, Texas A&M University at Qatar.
Lecture: "Thermodynamics of protein solutions: from science to chemical engineering" **Pedro de Alcântara Pessoa Filho**, *Universidade de São Paulo (USP), Brazil*
- 17:00

Poster Session + Coffee Break

Chair: *Jean Noel Jaubert, Universite de Lorraine, Nancy, France*

- 17:30 Oral Presentations.
- 17:30-17:45 Simultaneous multiphase flash and stability analysis calculations including hydrates
Iuri Soter Viana Segtovich, Amaro Gomes Barreto Jr., Frederico Wanderley Tavares
UFRJ - Universidade Federal do Rio de Janeiro, Brazil

- 17:45-18:00 Estimation of the uncertainty of predicted thermophysical property data
M. Shacham¹, G.St. Cholakov², N. Brauner³, R. P. Stateva⁴
¹Chemical Engineering Dept./Ben-Gurion University of the Negev, Israel
²University Chem.Technol. Metall., Sofia, Bulgaria
³School of Engineering, Tel-Aviv University, Israel
⁴Institute of Chemical Engineering, Bulgarian Acad. Sciences, Sofia, Bulgaria
- 18:00-18:15 Phase behavior of 1-alkyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide ionic liquids and alkanes from a Group-Contribution Equation of State
Emilio J. González¹, Susana B. Bottini², and Eugénia A. Macedo³
¹Department of Chemical Engineering, Complutense University, Madrid, Spain
²PLAPIQUI, Universidad Nacional del Sur-CONICET, Bahía Blanca, Argentina
³Faculdade de Engenharia da Universidade do Porto, Portugal
- 18:15-18:30 Employing a SAFT equation of state to obtain force fields for use in Coarse-Grained molecular simulations
George Jackson, Amparo Galindo, Claire S. Adjiman and Erich A. Müller¹
 Imperial College London - Dept. Chemical Engineering, United Kingdom
- 18:30-18:45 Modification of ZIF-8 structures: the effect of metal atom exchange on structural and separation properties
Panagiotis G. Krokidas¹, Marcelo Castier¹, Hae-Kwon Jeong² and Ioannis G. Economou¹
¹Texas A&M University at Qatar, Doha, Qatar
²Texas A&M University, Artie McFerrin Department of Chemical Engineering, USA
- 18:45-19.00 Including dispersive interactions in the F-SAC model
Guilherme Braganholo Flôres, Paula Bettio Staudt, Rafael de Pelegrini Soares
 Chemical Engineering Department, Federal University of Rio Grande do Sul, Brazil
- 19:00 End of work session
- 21:00 *Gala Dinner*
- 24:00 *Fireworks from the Santa Bárbara Castle*

TUESDAY, 30 June

Chair: *Theo de Loos, Delft University of Technology, Netherlands*

- 9:00 **Plenary Lecture: “Classical Thermodynamic Insights into Some Biochemical Processes”**
Stanley I. Sandler, University of Delaware, USA
- 9:45 Oral Presentations.
- 9:45-10:00 Thermodynamic modeling of new generation fuels
Mariana González Prieto, Francisco A. Sánchez and Selva Pereda
 Planta Piloto de Ingeniería Química (PLAPIQUI - UNS - CONICET), Argentina
- 10:00-10:15 Chemical potentials, activity coefficients and solubility in aqueous NaCl solutions: prediction by polarizable force fields
F. Moucka, W. R. Smith, I. Nezbeda
 J. E. Purkinje University, Canada
- 10:15-10:30 Characterization of the Global Phase Behaviour of Binary Mixtures: H₂S + CH₄, H₂S + CO₂ and CH₄ + CO₂ using the SAFT- γ Mie approach and molecular simulations
José Matías Garrido¹, José Manuel Míguez³, Felipe J. Blas², Andrés Mejía¹, Thomas Lafitte⁴, Manuel M. Piñeiro⁵
¹Universidad de Concepción, Chile
²Universidad de Huelva, Spain
³Université de Pau et des Pays de l'Adour, France
⁴Process Systems Enterprise Ltd., United Kingdom
⁵Universidad de Vigo, Spain

10:30-10:45	<p>Thermodynamic properties and phase equilibria of water from a polarizable intermolecular potential <i>I. Shvab and Richard J. Sadus</i> <i>Swinburne University of Technology, Australia</i></p>
10:45-11:00	<p>Predictive capability of the PC-SAFT equation of state and its polar extensions for liquid-liquid equilibria in systems containing γ-valerolactone <i>Martin Klajmon, Karel Reháč, Maja Matoušová, Pavel Morávek</i> <i>University of Chemistry and Technology, Prague, The Czech Republic</i></p>
11:00	<hr/> <p>Poster Session + <i>Coffee Break</i></p> <hr/>
<p>Chair: <i>Andrés Mejía, Universidad de Concepción, Chile</i></p>	
11:30	<p>Oral Presentations.</p>
11:30-11:45	<p>Comparison between different materials for CO₂ capture in a post-combustion stream <i>Daniel Bahamon and Lourdes F. Vega</i> <i>MATGAS Research Center, Spain</i></p>
11:45-12:00	<p>Thermodynamics for energy and sustainability. <i>Wolfgang Arlt and Karsten Müller</i> <i>University of Erlangen-Nuremberg, Chemical Engineering (CBI), Germany</i></p>
12:00-12:15	<p>A new investigation on effect of resin to asphaltene ratio on asphaltene precipitation <i>Taraneh Jafari Behbahani, Cyrus Ghotbi and Vahid Taghikhani</i> <i>Sharif University of Technology, Iran</i></p>
12:15-12:30	<p>Application of undefined mixture correlations and FTIR-PLS method to predict thermodynamic properties of hydroxyl group rich Kukersite oil shale derived “synthetic oils” <i>Zachariah S. Baird, Oliver Järvik and Vahur Oja</i> <i>Department of Chemical Engineering / Tallinn University of Technology, Estonia</i></p>
12:30-12:45	<p>Thermodynamic criteria for the selection of working substances in energy efficient process design <i>Karsten Müller and Wolfgang Arlt</i> <i>Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany</i></p>
12:45-13:00	<p>A new simple and efficient flash algorithm for T-V specifications <i>Martin Cismondi¹, Jorge Ourique², PapaMatar Ndiaye³ and Frederico W. Tavares^{3,4}</i> ¹<i>IDTQ-PLAPIQUI (Universidad Nacional de Córdoba, CONICET)</i> ² <i>Departamento de Engenharia Química. Universidade Federal Fluminense, Brazil.</i> ³ <i>Escola de Química – Universidade Federal do Rio de Janeiro, Brazil.</i> ⁴ <i>Programa de Engenharia Química/COPPE – Universidade Federal do Rio de Janeiro, Brazil</i></p>
13:00-13:15	<p>Recovery of carbohydrates from ionic liquids by precipitation with antisolvents <i>Aristides P. Carneiro¹, Oscar Rodríguez² and Eugénia A. Macedo¹</i> ¹<i>Faculdade de Engenharia, Universidade do Porto, Portugal</i> ²<i>University of Santiago de Compostela, Spain</i></p>
13:15-13:30	<p>Recovery process of condensable by-products from torrefaction of lignocellulosic biomass <i>M. Detcheberry, P. Destrac, J-S. Condoret and X-M. Meyer.</i> <i>Université de Toulouse ; INPT, UPS ; Laboratoire de Génie Chimique, France</i></p>
13:30	<hr/> <p><i>Lunch</i></p> <hr/>

Chair: *Eugenia Macedo, Universidade do Porto, Portugal*

- 15:00 Oral Presentations.
- 15:00-15:15 Application of CAPEC Lipids Property Databases in the synthesis and design of biorefinery networks
Maria-Ona Bertran, Larissa P. Cunico and Rafiqul Gani
CAPEC-PROCESS, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Denmark
- 15:15-15:30 Evaluation of different group contribution methods for simulating steam deacidification process
Simone M Silva¹, Roberta Ceriani² and Antonio J.A.Meirelles²
¹*University of Brasilia, Brazil*
²*University of Campinas, Brazil*
- 15:30-15:45 gSAFT: the use of advanced thermodynamic models in complex process modelling applications
Thomas Lafitte, Vasileios Papaioannou, Javier Rodriguez and Constantinos C Pantelides. Process Systems Enterprise, London, United Kingdom
- 15:45-16:00 MPinch: a software for heat exchanger networks synthesis
Mauro Ravagnani and Leandro Pavão
State University of Maringá, Brazil
- 16:15 **Plenary Lecture: "Thermodynamics of mixtures of ionic liquids and gases".**
Joan Brennecke, University of Notre-Dame, USA
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- 17:00 Poster Session + *Coffee Break*
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Chair: *Lourdes Vega, Carbueros Metálicos y MATGAS, Spain*

- 17:30 Oral Presentations.
- 17:30-17:45 Measurement and modelling of phase equilibria for the simulation of a biodiesel synthesis process
Romain Privat, Jean-Noël Jaubert, Niramol Juntarachat and Lucie Coniglio
ENSIC - LRGP - University of Lorraine, France
- 17:45-18:00 Comparison of the correlative abilities of semi-empirical models and a cubic equation of state on dyes and calix[4]arenes solubilities in SCCO₂ as illustrative examples
Jose AP Coelho¹, Greta P. Naydenova², Dragomir S. Yankov², and Roumiana P. Stateva²
¹*Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa and CIEQB, Instituto Superior de Engenharia de Lisboa, Portugal*
²*Institute of Chemical Engineering, Bulgarian Academy of Sciences, Sofia, Bulgaria*
- 18:00-18:15 Modeling of the binodal curve of ionic liquid/salt systems
Enrique Alvarez-Guerra¹, Sónia P.M. Ventura², Manuel Alvarez-Guerra¹, João A.P. Coutinho² and Angel Irabien¹
¹*Universidad de Cantabria, Dpto. de Ingenierías Química y Biomolecular, Spain*
²*Departamento de Química, CICECO, Universidade de Aveiro, Portugal*
- 18:15-18:30 Melting point depression effect with CO₂ in high melting temperature cellulose dissolving ionic liquid
Joana M. Lopes¹, Francisco A. Sánchez², S. Belén Rodríguez Reartes², M^a Dolores Bermejo¹, Ángel Martín¹ and M^a José Cocero¹
¹*Department of Chemical Engineering and Environmental Technology, Valladolid University, Spain*
²*Planta Piloto de Ingeniería Química (PLAPIQUI-UNS-CONICET), Bahía Blanca, Argentina*
- 18:30-18:45 Butanol–water partitioning for three 2-hydroxyethylammonium based ionic liquids at 293.15, 313.15 and 333.15 K
Isabela Sales¹, Karina Amorim¹, Simão P. Pinho² and Silvana Mattedi¹
¹*Federal University of Bahia, Brazil*
²*Polytechnic Institute of Bragança, Bragança, Portugal*

- 18:45-19:00 Solution of silk in ionic liquids by ultrasound irradiation to obtain regenerated silk fibroin nanoparticles
M. G. Montalbán, R. Trigo, M. Collado-González, F. Guillermo Díaz Baños, Antonio Abel Lozano-Pérez and G. Villora
University of Murcia, Spain
- 19:00 End of work session

WEDNESDAY, 1 July

Chair: *Silvana Mattedi, Universidade Federal da Bahia, Brazil*

- 9:00 **Plenary Lecture: "On fictional and Nonfictional Phase Equilibrium Computations".**
Marcelo Zabaloy, PLAPIQUI, Universidad Nacional del Sur, Argentina
- 9:45 Oral Presentations.
- 9:45-10:00 Playing with ammonium-based bistriflamide ionic liquids to understand their interactions with molecular solvents
André Mão de Ferro¹, Patrícia M. Reis¹, Anabela J. L. Costa¹, Carlos E. S. Bernardes², Karina Shimizu², José N. Canongia Lopes^{1,2}, José M. S. S. Esperança¹ and Luís Paulo N. Rebelo¹
¹*Instituto de Tecnologia Química e Biológica, Universidade Nova de Lisboa, Portugal*
²*Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, Portugal*
- 10:00-10:15 Phase equilibria and self-aggregation behaviour of fluorinated ionic liquids in water
Felix Llovell¹, Ana B. Pereira², João M. M. Araújo², Luis Paulo N. Rebelo², Manuel M. Piñeiro³ and Lourdes F. Vega¹
¹*MATGAS 2000 AIE, Barcelona, Spain*
²*Instituto de Tecnologia Química e Biológica, Universidade Nova de Lisboa, Portugal*
³*Universidade de Vigo, Spain*
- 10:15-10:30 Assessing gas separation of greenhouse and acid gases with ionic liquids.
Felix Llovell¹, Mariana B. Oliveira², João A. P. Coutinho² and Lourdes F. Vega¹
¹*MATGAS 2000 AIE, Barcelona, Spain*
²*Universidade de Aveiro, Portugal*
- 10:30-10:45 Phase behavior and optimization of the process parameters effect on Polystyrene recycling using natural terpenes and CO₂
Cristina Gutiérrez, M^a Teresa García, Eulalio Gracia, Ignacio Gracia, Antonio de Lucas and Juan Francisco Rodríguez
University of Castilla-La Mancha, Spain
- 10:45-11:00 Effect of the estimated critical properties of an ionic liquid on the modeling with equation of states of thermophysical properties and CO₂ solubility
Cor J. Peters, Maaike C. Kroon and María Teresa Mota Martínez Eindhoven
University of Technology, The Netherlands
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- 11:00 Poster Session + Coffee Break

Chair: *Ana Soto, Universidad de Santiago de Compostela, Spain*

- 11:30 Oral Presentations.
- 11:30-11:45 Phase equilibrium studies of electrolytes and precursors in carbon dioxide and hydrofluorocarbons for supercritical fluid electrodeposition and production of nanomaterials
Jie Ke, Xue Han, Norhidayah Suleiman and Michael W. George
University of Nottingham, United Kingdom

11:45-12:00	<p>High pressure vapor-liquid equilibria for binary methane+protic ionic liquid based on propionate anions <i>Luana M.C. Oliveira¹, Fábila R.G. Ribeiro², Dheiver F. Santos¹, A. C. Feirhmann², Vladimir F. Cabral², Lúcio Cardozo-Filho² and S. Mattedi¹</i> ¹Federal University of Bahia, Brazil ²State University of Maringá, Brazil</p>
12:00	<p>Closing Lecture: "Property model-data based chemical product-process design". <i>Rafiqul Gani, Technical University of Denmark, Denmark.</i></p>
12:45	<p>Closing Ceremony</p> <hr/>
13:15	<p><i>Lunch</i></p> <hr/>