

Conference Program



**X Iberoamerican Conference on Phase
Equilibria and Fluid Properties
for Process Design**
June 28-July 1, 2015 - Alicante (SPAIN)





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WELCOME

On behalf of the Organizing Committee, we welcome you to the X Iberoamerican Conference on Phase Equilibria and Fluid Properties for Process Design EQUIFASE 2015. It is our greatest pleasure to host all of you in the Mediterranean city of Alicante, with its long sandy beaches and mild climate.

We are very pleased for the interest shown in this conference, resulting in the large number of fine contributions we have received from many parts of the world.

The scientific program provides, as previous editions of the EQUIFASE Congress, an excellent opportunity for participants to exchange new ideas and information on many important issues in phase equilibria and fluid properties. The program includes high-standard plenary lectures. We want to express our gratitude to the invited speakers for their contribution to the excellence of the meeting.

We wish also thank the International Scientific Committee for their support in all the aspects of the event. We also deeply appreciate the participation of leader companies and government agencies and institutions as sponsors of this conference.

We wish you all a fruitful meeting. Welcome to Alicante and many thanks for making EQUIFASE 2015 possible!

Antonio and Vicente



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International Committee

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ABOUT EQUIFASE

In April 1983, the third International Conference on Fluid Properties and Phase Equilibria for Chemical Process Design took place in Callaway Gardens, Georgia, USA. This event stimulated the Latin American participants to organize an International Course on the Thermodynamics of Phase Equilibria in Bahía Blanca (Argentina), in July 1984. This course brought a large number of participants from industry and universities, giving the chance to program scientific and technical interchange activities in the field of vapor–liquid equilibrium for process design. This was the first step for the series of EQUIFASE Conferences reported below, being held periodically:

EQUIFASE 1987:	Concepción, Chile
EQUIFASE 1990:	Salvador de Bahía, Brazil
EQUIFASE 1992:	Oaxaca, México
EQUIFASE 1995:	Caracas, Venezuela
EQUIFASE 1999:	Vigo, Spain
EQUIFASE 2002:	Foz de Iguazu, Brazil and Argentina
EQUIFASE 2006:	Morelia, Mexico
EQUIFASE 2009	Praia da Rocha, Portugal
EQUIFASE 2012	Puerto Varas, Chile
EQUIFASE 2015	Alicante, Spain

The general purpose of the EQUIFASE Conference is to promote the Scientific and Technologic exchange between people from both the academic and the industrial environment from the European and American Continents in the field of Phase Equilibria and Thermodynamic Properties for the Design of Chemical Processes. The main topics of this Conference are related to measurement, modeling, prediction and simulation of physical–chemical properties concerning product and process design.



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EQUIFASE 2015

Alicante is a Spanish city located on the Mediterranean coast. It has an arid Mediterranean climate, with mild temperatures all year long and little rain. Alicante is a modern city with a primary focus on tourism, but also a special interest in industry and commerce. It offers not only a great variety of services, but also a wide range of cultural activities, with its museums, its festivals and its nature areas. Alicante is a perfect city for spending a few pleasantly relaxing days.

EQUIFASE 2015 is held at the Meliá Hotel, one of the city's most iconic hotels, which is located between Postiguet Beach and Alicante Marina, near the well-known Paseo de la Explanada de España, the historic and commercial center of the city and Santa Bárbara Castle.

SCOPE AND TOPICS

1. Measurement of Thermodynamic Properties. Phase Equilibria and Chemical Equilibria
2. Theory and Modelling: Statistical Thermodynamic, Equations of State, Activity Coefficient Models, Molecular Simulation and Multiscale Simulation
3. Alternative solvents. Supercritical fluids. Ionic liquids
4. Energy. Gas and oil. Petrochemicals. Environment and sustainability
5. Biomolecules and Biotechnology
6. Product and Process Design. Databases and Software
7. Education



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ESTEBAN A. BRIGNOLE AWARD

This will be the first edition of the Esteban A. Brignole Award, recognized as the most prominent figure in the area of Applied Thermodynamics in Latin America. His major research contributions are the pioneering work on molecular design of solvents and the novel integration of rigorous thermodynamic methods to process engineering, which have gained him international recognition.

As the person who gives its name to the prize, the distinguished with the Esteban A. Brignole Award are expected to combine technical excellence with selfless service to promote progress, innovation, and collaboration. The members of the International Scientific Committee of EQUIFASE 2015 have awarded this prize to *Pedro de Alcántara Pessoa Filho*, Professor in the Chemical Engineering Department, University of Sao Paulo, Brazil. Professor Pedro de Alcántara Pessoa Filho is awarded for the high quality standards in his scientific work, by building bridges of approximation between different research groups, by working as an editor for several iberoamerican and international scientific and academic journals and by his passion for scientific progress and innovation.

SPECIAL ISSUE OF FLUID PHASE EQUILIBRIA

The Editors of Fluid Phase Equilibria have arranged for publication (after peer-reviewed) of the EQUIFASE 2015 Conference Proceedings, as a Special Issue of FPE. Only authors of selected papers will be invited to submit a manuscript. Selection will take place during the conference by the guest editors and the FPE handling editors.

- Editors: Theo de Loos and Ana Soto
- Guest Editors: Antonio Marcilla and Vicente Gomis

Scientific Program

SCIENTIFIC PROGRAM – EQUIFASE 2015

SUNDAY, 28 June

16:00	Registration
19:30	Welcome reception and <i>Cocktail</i>

MONDAY, 29 June

9:00	Conference Presentation
9:10	<i>In memoriam</i> Hugo Segura Andrés Mejía, Universidad de Concepción, Chile

Chair: *Cor Peters, The Petroleum Institute, Abu Dhabi, UAE*

9:15 (PL-1)	Inaugural Lecture: “Modelling water in computer simulations” <i>Carlos Vega, Complutense University of Madrid, Spain</i>
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10:00 Oral Presentations

10:00-10:15 (O-01)	Description of solid-liquid equilibria in complex mixtures involved in the acid processing of aluminosilicate ores <i>Teyssier Angélique^{1,2}, Jean-Michel Schmitt¹, Christelle Goutaudier²</i> ¹ AREVA, BG Mines, France ² Laboratoire des Multimatériaux et Interfaces, UMR CNRS 5615, Université Claude Bernard Lyon 1, France
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10:15-10:30 (O-02)	Improved correlations for viscosity of naphthenic crude oils <i>Krishnaswamy Rajagopal, Luciana L. de Pinho Rolemberg de Andrade</i> <i>Escola de Química / Univ. Federal do Rio de Janeiro, Brazil</i>
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10:30-10:45 (O-03)	Solid-liquid equilibrium of CuSO₄-H₂SO₄-seawater system <i>Francisca Justel, Yecid Jiménez, María Elisa Taboada</i> <i>Universidad de Antofagasta, Chile</i>
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10:45-11:00 (O-04)	Solid-solid-liquid equilibrium of lipidic ternary mixtures <i>Guilherme J. Maximo¹, Rafael T. Aquino², Antonio J. A. Meirelles¹, Mariana C. Costa²</i> ¹ School of Food Engineering, University of Campinas, Brazil ² School 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 (O-05)	High-pressure densities and surface tensions of binary and ternary system containing carbon dioxide + n-alkanes <i>Constanza Cumicheo, Marcela Cartes and Andres Mejia</i> <i>Dpto. Ingeniería Química, Universidad de Concepción, Chile</i>
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- 11:45-12:00 (O-06) **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 (O-07) **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 (O-08) **Gas hydrate phase behavior in presence of organics and electrolytes**
Khalik M. Sabil¹, Cor J. Peters²
¹Heriot Watt University, Eindhoven University of Technology, The Netherlands
²The Petroleum Institute, Abu Dhabi, UAE
- 12:30-12:45 (O-9) **Comments on the correlation of liquid-vapour and liquid-liquid-vapour equilibrium data**
Antonio Marcilla, Juan Antonio Reyes-Labarta, María del Mar Olaya
Chemical Engineering Department, University of Alicante, Spain
- 12:45-13:00 (O-10) **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 (O-11) **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.
¹Institute of Multidisciplinary Research for Advanced Materials (IMRAM) Japan
²Institute of Environmental Engineering of the Polish Academy of Sciences, Poland
³COSMOlogic 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 (O-12) **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 Juntarachat¹ and Christophe Coquelet²
¹*ENSIC - LRGP - University of Lorraine, France*
²*CTP-Mines Paristech, France*
- 15:15-15:30 (O-13) **Extension of the Soft-SAFT thermodynamic model to derivative and transport properties**
Felix Llovell, Lourdes F. Vega
MATGAS 2000 AIE, Spain
- 15:30-15:45 (O-14) **A 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 (O-15) **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 (O-16) **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 (PL-2) **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
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- 17:00 Poster Session + Coffee Break
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Chair: *Jean Noel Jaubert, Universite de Lorraine, Nancy, France*

- 17:30 Oral Presentations
- 17:30-17:45 (O-17) **Simultaneous multiphase flash and stability analysis calculations including hydrates**
Juri Soter Viana Segtovich, Amaro Gomes Barreto Jr., Frederico Wanderley Tavares
UFRJ - Universidade Federal do Rio de Janeiro, Brazil
- 17:45-18:00 (O-18) **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 (O-19) **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 (O-20) **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 (O-21) **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 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 (PL-3)

Plenary Lecture: “Classical Thermodynamic Insights into Some Biochemical Processes”

Stanley I. Sandler, University of Delaware, USA

9:45

Oral Presentations

9:45-10:00 (O-22)

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 (O-23)

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 (O-24)

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

10:30-10:45 (O-25)

Thermodynamic properties and phase equilibria of water from a polarizable intermolecular potential

I. Shvab and Richard J. Sadus

Swinburne University of Technology, Australia

10:45-11:00 (O-26)

Predictive capability of the PC-SAFT equation of state and its polar extensions for liquid-liquid equilibria in systems containing γ -valerolactone

Martin Klajmon, Karel Reháč, Maja Matoušová, Pavel Morávek

University of Chemistry and Technology, Prague, The Czech Republic

11:00

Poster Session + Coffee Break

Chair: *Andrés Mejía, Universidad de Concepción, Chile*

- 11:30 Oral Presentations
- 11:30-11:45 (O-27) **Comparison between different materials for CO₂ capture in a post-combustion stream**
Daniel Bahamon and Lourdes F. Vega
MATGAS Research Center, Spain
- 11:45-12:00 (O-28) **Thermodynamics for energy and sustainability**
Wolfgang Arlt and Karsten Müller
University of Erlangen-Nuremberg, Chemical Engineering (CBI), Germany
- 12:00-12:15 (O-29) **A new investigation on effect of resin to asphaltene ratio on asphaltene precipitation**
Taraneh Jafari Behbahani, Cyrus Ghotbi and Vahid Taghikhani
Sharif University of Technology, Iran
- 12:15-12:30 (O-30) **Application of undefined mixture correlations and FTIR-PLS method to predict thermodynamic properties of hydroxyl group rich Kukersite oil shale derived “synthetic oils”**
Zachariah S. Baird, Oliver Järviik and Vahur Oja
Department of Chemical Engineering / Tallinn University of Technology, Estonia
- 12:30-12:45 (O-31) **Thermodynamic criteria for the selection of working substances in energy efficient process design**
Karsten Müller and Wolfgang Arlt
Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany
- 12:45-13:00 (O-32) **A new simple and efficient flash algorithm for T-V specifications**
Martin Cismondi¹, Jorge Ourique², PapaMatar Ndiaye³ and Frederico W. Tavares^{3,4}
¹IDTQ-PLAPIQUI (Universidad Nacional de Córdoba, CONICET)
²Departamento de Engenharia Química. Universidade Federal Fluminense, Brazil.
³Escola de Química – Universidade Federal do Rio de Janeiro, Brazil.
⁴Programa de Engenharia Química/COPPE – Universidade Federal do Rio de Janeiro, Brazil

- 13:00-13:15 (O-33) **Recovery of carbohydrates from ionic liquids by precipitation with antisolvents**
Aristides P. Carneiro¹, Oscar Rodríguez² and Eugénia A. Macedo¹
¹Faculdade de Engenharia, Universidade do Porto, Portugal
²University of Santiago de Compostela, Spain
- 13:15-13:30 (O-34) **Recovery process of condensable by-products from torrefaction of lignocellulosic biomass**
M. Detcheberry, P. Destrac, J-S. Condoret and X-M. Meyer.
Université de Toulouse ; INPT, UPS ; Laboratoire de Génie Chimique, France
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- 13:30 Lunch
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- Chair:** Eugenia Macedo, Universidade do Porto, Portugal
- 15:00 Oral Presentations
- 15:00-15:15 (O-35) **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 (O-36) **Evaluation of different group contribution methods for simulating steam deacidification process**
Simone M Silva¹, Roberta Ceriani² and Antonio J.A.Meirelles²
¹University of Brasilia, Brazil
²University of Campinas, Brazil
- 15:30-15:45 (O-37) **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 (O-38) **MPinch: a software for heat exchanger networks synthesis**
Mauro Ravagnani and Leandro Pavão
State University of Maringá, Brazil
- 16:15 (PL-4) **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 (O-39) **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 (O-40) **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
¹Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa and CIEQB, Instituto Superior de Engenharia de Lisboa, Portugal
²Institute of Chemical Engineering, Bulgarian Academy of Sciences, Sofia, Bulgaria

18:00-18:15 (O-41) **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
¹Universidad de Cantabria, Dpto. de Ingenierías Química y Biomolecular, Spain
²Departamento de Química, CICECO, Universidade de Aveiro, Portugal

18:15-18:30 (O-42) **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
¹Department of Chemical Engineering and Environmental Technology, Valladolid University, Spain
²Planta Piloto de Ingeniería Química (PLAPIQUI-UNS-CONICET), Bahía Blanca, Argentina

18:30-18:45 (O-43) **Butanol–water partitioning for three 2-hydroxyethylamonium based ionic liquids at 293.15, 313.15 and 333.15 K**
Isabela Sales¹, Karina Amorim¹, Simão P. Pinho² and Silvana Mattedi¹
¹Federal University of Bahia, Brazil
²Polytechnic Institute of Bragança, Bragança, Portugal

- 18:45-19:00 (O-44) **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 (PL-5) **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 (O-45) **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 (O-46) **Phase equilibria and self-aggregation behaviour of fluorinated ionic liquids in water**
Felix Llovell¹, Ana B. Pereiro², 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 (O-47) **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 (O-48) **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 (O-49) **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, Maaïke C. Kroon and María Teresa Mota Martínez
Eindhoven University of Technology, The Netherlands
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- 11:00 **Poster Session + Coffee Break**
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- Chair:** *Ana Soto, Universidad de Santiago de Compostela, Spain*
- 11:30 **Oral Presentations**
- 11:30-11:45 (O-50) **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 (O-51) **High pressure vapor-liquid equilibria for binary methane+protic ionic liquid based on proprionate anions**
Luana M.C. Oliveira¹, Fábïa R.G. Ribeiro², Dheiver F. Santos¹, A. C. Feirhmann², Vladimir F. Cabral², Lúcio Cardozo-Filho² and S. Mattedi¹
¹*Federal University of Bahia, Brazil*
²*State University of Maringá, Brazil*
- 12:00 (PL-6) **Closing Lecture: "Property model-data based chemical product-process design"**
Rafiqul Gani, Technical University of Denmark, Denmark
- 12:45 **Closing Ceremony**
-
- 13:15 **Lunch**
-

Poster Session

POSTER SESSION – EQUIFASE 2015

TOPIC 1. Measurement of Thermodynamic Properties. Phase Equilibria and Chemical Equilibria

- P-01 **Density measurements under pressure of di-isopropyl ether + 2-butanol at temperatures up to 393.15 K and at pressures up to 100 MPa**
Mohamed Dakkach², Fatima E. M. Alaoui³, Fernando Aguilar¹, Eduardo Montero¹
¹*Escuela Politécnica Superior, Universidad de Burgos, Spain*
²*Faculty of Sciences, Abdelmalek Essaâdi University, Morocco.*
³*Ecole Nationale des Sciences Appliquées d'El Jadida, Chouaïb Doukkali University, Morocco*
- P-02 **Enzymatic reaction in two phase systems: prediction of equilibrium conversion at equilibrium**
Jose A. Scilipoti, Claudia Nioi, Séverine Camy, Jean-Stéphane Condoret
Université de Toulouse, CNRS-INPT-UPS, Laboratoire de Génie Chimique, France
- P-03 **Aqueous two-phase system of poly(ethylene glycol) 4000 and sodium molybdate at different temperatures**
Katherine Muñoz, Islamán Bannura, Yahaira Barrueto, Katiuska Garnica, Yecid P. Jiménez
Universidad de Antofagasta, Chile
- P-04 **Thermodynamic analysis of ethanol and 1-propanol dehydration via extractive distillation**
Jordi Pla-Franco, Estela Lladosa, Sonia Loras and Juan B. Montón
Dpto. Ingeniería Química, Universitat de València, Spain
- P-05 **Liquid-liquid equilibria for ternary mixture of [hmim⁺][NTf₂⁻] + n-hexane + an organic compound involved in the kinetic resolution of *rac*-2-pentanol**
M. G. Montalbán, C. L. Bolívar, R. Trigo, M. Collado-González, F. Guillermo Díaz Baños and G. Vllora
University of Murcia, Spain
- P-06 **Evaluation of diethyl carbonate and methyl isobutyl ketone as entrainers in 1-hexene + n-hexane mixtures**
Beatriz Marrujo¹, Jordi Pla-Franco², Sonia Loras²
¹*Universidad del Zulia, Maracaibo, Venezuela*
²*Universitat de València, Spain*
- P-07 **Isobaric vapor-liquid equilibrium of binary mixtures HFE 7500 + di-isopropyl ether**
Natalia Muñoz, Adil Srhiyer, Eduardo Montero, Fernando Aguilar
Escuela Politécnica Superior, Universidad de Burgos, Spain

- P-08 **Excess molar Gibbs energies of heptan-2-one + 1,4-dichlorobutane or + 1,6-dichlorohexane. Measurements and predictions**
Ouahiba Tafat-Igoudjilene, A. Ait Kaci¹, J. Jose²
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²*Laboratoire de Chimie Analytique I, Université Claude Bernard, France*
- P-09 **Development of an innovative process of extraction of high purity hydrazine : exploitation of phase equilibria**
Anne-Julie Bougrine¹, Clelia Betton¹, Guy Jacob², Henri Delalu¹
¹*Laboratoire Hydrazines et Composés Energétiques Polyazotés Université Claude Bernard Lyon 1, France*
²*SAFRAN-HERAKLES-Centre de Recherches du Bouchet, France*
- P-10 **Excess molar enthalpies for binary mixtures of N and/or O-heterocyclic compounds with octane isomers at 308.15 K and atmospheric pressure. Experimental results and DISQUAC model analysis**
Farid Brahim Belaribi, Nadia Abdouche, Assia Boussebissi, Ghénima Boukais-Belaribi
Université des Sciences et de la Technologie Houari Boumediene. Algérie
- P-11 **Binary solid-liquid equilibrium of trimyristin + fatty acids**
Flávio Cardoso de Matos, Mariana Conceição da Costa, Eduardo Augusto Caldas Batista
University of Campinas, Brazil
- P-12 **Calorimetric study on the influence of branched-chain fatty alcohol esters as inhibitors of solid-liquid equilibrium of ethylic biodiesel components**
Maria Dolores Robustillo Fuentes¹, Antonio Jose De Almeida Meirelles², Pedro De Alcântara Pessôa Filho¹
¹*Universidade de São Paulo, Brazil*
²*University of Campinas, Brazil*
- P-13 **Phase equilibrium and properties of lithium hydroxide in water + methanol and different temperatures**
Teófilo Graber¹, Elsa Flores², Maria Elisa Taboada¹
¹*Universidad de Antofagasta, Chile*
²*CICITEM, Chile*
- P-14 **Comparison of two indirect methods for determining liquid-liquid equilibria of sunflower seed oil (1) + n-hexanal or 2-nonenal (2) + anhydrous ethanol (3) at 293.2 K**
Perci Homrich, Roberta Ceriani
University of Campinas, Brazil

- P-15 **Temperature and water content effect on viscosity and conductivity of protic ionic liquids based on N-methyl-2-hydroxyethylammonium cation**
Gala Rosales, Fabio Costa, Flora Alves, Jaime Boaventura and Silvana Mattedi
Federal University of Bahia, Brazil
- P-16 **Thermophysical characterization of peloids from Chilca (Perú) for therapeutics uses**
Carmen P. Gómez, Lourdes Mourelle, Cristina Fernández, Dolores Fernandez-Marcos, José Luis Legido
University of Vigo, Spain
- P-17 **Solid-liquid equilibrium in lysozyme precipitation with biodegradable salts**
José Sebastián López Vélez. Pedro de Alcântara Pessôa Filho
Universidade de São Paulo, Brazil
- P-18 **Surface tension for the ternary system dimethyl carbonate + p-xylene+ n-octane from 288.15 K – 308.15 K**
Ana Gayol¹, Lidia Casás², Raquel E. Martini³, Alfonsina E. Andreatta⁴, José Luis Legido¹
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⁴*Universidad Tecnológica Nacional Facultad Regional San Francisco, Córdoba, Argentina*
- P-19 **Experimental and theoretical study of surface tension and density of 1,2-dimethylbenzene with alkanes at 298.15K**
Alfonsina E. Andreatta³, Raquel E. Martini², José L. Legido¹, Lidia Casás⁴
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P-20 Phase equilibria of glycols and hydrocarbon: experimental measurements and modeling with the GCA-EoS

Mariana González Prieto¹, Mark D. Williams-Wynn², Indra Bahadur², Francisco A. Sánchez¹, Selva Pereda¹, Amir H. Mohammadi², Deresh Ramjugernath²

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P-21 The effect of propanol on the solubility of acidic copper sulfate solutions at 298.15K

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P-22 Use of distilled crude oil fractions to describe phase behavior of crude oil in carbon dioxide

Marcos A. Lucas, Rafael B. M. Nunes, Cláudio Dariva, Montserrat F. Heredia, Alexandre F. Santos, Elton Franceschi, Gustavo R. Borges

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P-23 Synthesis and solubility measurement of 2-methyl-1,4-naphthoquinone (menadione) derivatives in supercritical carbon dioxide

Adolfo L. Cabrera¹, Flavia C. Zacconi², José M. del Valle² and Juan C. de la Fuente²

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P-24 Vapor + liquid equilibria at high-pressure for ternary systems (e)-2-hexenal or hexanal + carbon dioxide + water: measure of partition coefficients

Arturo Bejarano¹, Pablo López², José M. de Valle¹, and Juan C. de la Fuente³

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³*Centro regional de estudios en alimentos saludables CREAS, Chile*

- P-25 **Solubility of carbon dioxide in systems containing MEG/Water/CaCO₃**
Fabiane Serpa, Reginaldo Vidal, João Amaral-Filho, Jailton Nascimento, Camila Figueiredo, Giancarlo Salazar-Banda, Elton Franceschi, Gustavo Borges and Cláudio Dariva
Universidade Tiradentes, Brazil
- P-26 **Analysis of surface tension variation with temperature for n-alkane and 1-alkanol**
M.M Mato, J. Cerqueiro, J. García, J.L. Legido
Universidad de Vigo, Spain
- P-27 **The liquid-liquid equilibrium for a ternary mixture composed of water, sulfolane and n-hexane at temperatures of 293.15, 303.15 and 313.15K**
Fernanda Ganem, João Paulo Santos, Luiz Mário Nelson Góis and Silvana Mattedi
Federal University of Bahia, Brazil
- P-28 **Study of temperature and water content effect on viscosity, density and speed of sound for protic ionic liquids based on bis(2-hydroxy-ethylammonium) cation**
João Paulo Santos, Dheiver F. Santos, Fábio Costa, Alexander Zimmermann, Jaime Boaventura and Silvana Mattedi
Federal University of Bahia, Brazil
- P-29 **Coupled processes as the basis of biodiesel production**
Alexandra Golikova, Anna Sadaeva, Maria Toikka and Maya Trofimova
Saint-Petersburg State University, Russia
- P-30 **High pressure phase behavior of carbon dioxide, 2-propanone and 4-nitrobenzaldehyde**
Técio Santos Bastos¹, Gustavo Rodrigues Borges¹, Cláudio Dariva¹, Reinaldo Bazito², Refael Francisco Cassaro², Elton Franceschi¹
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²Instituto de Química, Universidade de São Paulo, Brazil
- P-31 **The salt effect on the solubility of glycylglycine and n-acetyl-glycine**
Olga Ferreira, Yoselyn S. Santos, Ana M. Marafona, Mónica P. Gonçalves and Simao Pinho
Instituto Politécnico de Bragança (LSRE_IPB), Portugal
- P-32 **Measurement of ibuprofen - supercritical carbon dioxide phase equilibrium**
Antonio Montes, Clara Pereyra and Enrique J. Martínez de la Ossa
Department of Chemical Engineering and Food Technology, University of Cádiz, Spain

- P-33 **Determination of liquid-liquid-solid equilibrium data of the system water + 2-propanol + 1-undecanol at different temperatures and comparison with the system water + ethanol + 1-undecanol**
Vicente Gomis¹, M^a Dolores Saquete¹, Alicia Font¹, Nuria Boluda-Botella¹, Jorge García-Cano¹ and Kerry Davidson²
¹ *Department of Chemical Engineering. University of Alicante, Spain*
² *Department of Chemical & Process Engineering, University of Strathclyde, Scotland*
- P-34 **The use of heavy alcohols in the ethanol dehydration: liquid-liquid-solid equilibrium data of the ternary system water + ethanol + 1-undecanol at different temperatures**
Vicente Gomis¹, M^a Dolores Saquete¹, Alicia Font¹, Nuria Boluda-Botella¹, Jorge García-Cano¹ and Julie Crichton²
¹ *Department of Chemical Engineering. University of Alicante, Spain*
² *Department of Chemical & Process Engineering, University of Strathclyde, Scotland*
- P-35 **Determination of the vapor-liquid-liquid-solid equilibrium of water + NaCl + 1-butanol at 101.3 kPa**
Jorge García-Cano, Vicente Gomis, Juan Carlos Asensi.
Department of Chemical Engineering. University of Alicante, Spain

TOPIC 2. Theory and Modelling: Statistical Thermodynamic, Equations of State, Activity Coefficient Models, Molecular Simulation and Multiscale Simulation

- P-36 **Evaluating ionic Gibbs energy of hydration using the Q-electrolattice equation of state**
André Zuber¹ and Marcelo Castier²
¹ *State University of Maringá, Brazil*
² *Texas A&M University at Qatar, Qatar*
- P-37 **Thermodynamic properties of C₆₀ fullerene from an advanced perturbation theory**
Julio Largo and J. Ramón Solana
Departamento de Física Aplicada. Universidad de Cantabria, Spain
- P-38 **Binaries and ternaries phase diagrams for mixtures of vegetables oils, alcohols and co-solvents**
Kayo Santana, Sarah Arvelos, and Lucienne L. Romanielo
Universidade Federal de Uberlândia, Brazil
- P-39 **A new approach to modelling the equilibrium conditions of TBAB semi-clathrates formed in the presence of pure gases and gas mixtures**
Matthew Clarke and Marlon Garcia
University of Calgary, Canada

- P-40 **Molecular dynamics simulation studies of the interactions in amino acid-based ionic liquids**
Diana Ruivo¹, Karina Shimizu², José M.S.S. Esperança¹, José N. Canongia Lopes^{1,2}, Luís Paulo N. Rebelo¹
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²*Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, Portugal*
- P-41 **A modified multi-site occupancy model for heterogeneous surfaces**
Sarah Arvelos and Lucienne L. Romanielo
Universidade Federal de Uberlândia, Brazil
- P-42 **Activity coefficients of LiClO₄ in ionic liquid**
Jaime W. Morales
Escuela de Ingeniería Química/Pontificia Universidad Católica de Valparaíso, Chile
- P-43 **Molecular dynamics simulation of Henry's constant of CO₂ in ionic liquids using Multistate Bennett Acceptance Ratio**
Dheiver Santos¹, Guilherme Carneiro², Charles Abreu², Frederico W. Tavares², Silvana Mattedi¹
¹*Federal University of Bahia, Brazil*
²*Federal University of Rio de Janeiro, Rio de Janeiro, Brazil*
- P-44 **Development of a thermodynamic model for fluids confined in spherical pores**
Michelle D'Lima, Marcelo Castier
Texas A&M University at Qatar, Qatar
- P-45 **Molecular simulation of structural relaxation of asphaltene aggregates in presence of resin**
Toshimasa Takanohashi¹, Shinya Sato¹ and Ryuzo Tanaka²
¹*National Institute of Advanced Industrial Science and Technology, Japan*
²*Japan Petroleum Energy Center, Japan*
- P-46 **Characterization of the heterogeneous region of computed solid-fluid equilibrium isopleths**
Sabrina Belén Rodríguez-Reartes, Marcelo S. Zabaloy
Departamento de Ingeniería Química - Universidad Nacional del Sur, Argentina
- P-47 **A new reduction techniques for fast compositional reservoir simulation with cubic EoS**
Mehdi Assareh¹, Cyrus Ghotbi² Mahmoud Reza Pishvaie²
¹*School of Chemical Engineering, Iran University of Science and Technology, Tehran, Iran*
²*Department of Chemical and Petroleum Engineering, Sharif University of Technology, Tehran, Iran*

- P-48 **Calculation of complex phase equilibrium isotherms in ternary systems**
Gerardo O. Pisoni¹, Martín Cismondi², Lucio Cardozo-Filho¹, Marcelo S. Zabaloy³
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²*IDTQ- Grupo Vinculado PLAPIQUI – CONICET, Argentina*
³*Planta Piloto de Ing. Química/ Departamento de Ingeniería Química, UNS, CONICET, Argentina*
- P-49 **A New Parameterization for Cubic EoS from Single-Phase Properties**
David Santos, Márcio Paredes and Eduardo Lima
Universidade do Estado do Rio de Janeiro, Brazil
- P-50 **Thermodynamic modeling of speed of sound and density at high pressures for (tetralin/n-hexadecane) system with SAFT, PHCT and PFP equations of state**
Fábio Nascimento, Márcio Paredes and Fernando Pessoa
Universidade do Estado do Rio de Janeiro, Brazil
- P-51 **Evaluation of COSMO-RS for VLE prediction of the system 1,8-cineole+propan-1-ol**
José F. Martínez-López¹, Pascual Pérez¹, Elisa Langa², José S. Urieta¹, Ana M. Mainar¹
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²*Facultad de Ciencias de la Salud, Universidad San Jorge, Spain*
- P-52 **Direct detection of double retrograde behavior for equation of state models**
Juan I. Ramello¹, Juan M. Milanesio¹, Gerardo O. Pisoni², Martín Cismondi¹, Marcelo S. Zabaloy²
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- P-53 **Simultaneous ternary LLV and LV equilibrium correlation. modification of the NRTL equation for improved calculations**
Antonio Marcilla, Juan A. Reyes-Labarta and María del Mar Olaya.
Department of Chemical Engineering. University of Alicante, Spain
- P-54 **Modification of the NRTL equation for improved VLE calculations in ternary systems**
Antonio Marcilla, Juan A. Reyes-Labarta and María del Mar Olaya.
Department of Chemical Engineering. University of Alicante, Spain
- P-55 **Refreshing the relevance of analyzing the topology of the GM function in the phase equilibrium correlation data**
Antonio Marcilla, Juan A. Reyes-Labarta and María del Mar Olaya.
Department of Chemical Engineering. University of Alicante, Spain

P-56 Improved VLE and VLLE calculations in Azeotropic and Non-azeotropic systems (II). Effect of the vapor and total pressure

*Antonio Marcilla, Juan A. Reyes-Labarta and María del Mar Olaya
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TOPIC 3. Alternative solvents. Supercritical fluids. Ionic liquids

P-57 Study of the suitability of two ammonium based-ionic liquids for the extraction of benzene from its mixtures with aliphatic hydrocarbons

*Patricia F. Requejo, Elena Gómez, Noelia Calvar and Ángeles Domínguez
University of Vigo, Spain*

P-58 Spectroscopic studies of phase behaviour in nanopores: toward supercritical fluid electrodeposition

*Ashley Love, Xue-Han, Kie Jie and Michael George
University of Nottingham, United Kingdom*

P-59 Liquid-vapor equilibrium modeling of binary mixtures involving ionic liquids and supercritical fluids using two Gibbs Free Energy models

*Pedro Arce¹, Pedro Robles², Luis Cisternas²
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²University of Antofagasta, Chile*

P-60 Liquid-liquid equilibria of water + ethanol + 1-butyl-1-methylpyrrolidinium bis(trifluoromethanesulfonyl)imide ternary system

*Amparo Cháfer, Javier de la Torre, Estela Lladosa and Juan B. Montón
University of Valencia, Spain*

P-61 Prediction of liquid-liquid equilibrium for binary and ternary systems containing 1-alkyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide using the ASOG method

*Pedro Robles and Luis Cisternas
University of Antofagasta, Chile*

P-62 Toxicity of environmentally-friendly ionic liquids

*Nicole S. M. Vieira, Fátima Moscoso, Patrícia M. Reis, João M. M. Araújo,
José N. Canongia Lopes, Ana B. Pereiro, José M. S. S. Esperança, Luís Paulo
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P-63 Thermophysical characterization and partition properties of fluorinated ionic liquids

*Nicole S. M. Vieira¹, Patrícia M. Reis¹, João M. M. Araújo¹, Karina Shimizu²,
José N. Canongia Lopes^{1,2}, José M. S. S. Esperança¹, Ana B. Pereiro¹, Luís
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Lisboa, Portugal*

- P-64 **Apparent molar volumes of ionic liquids + methanol/ethanol at 298.15 K**
Rafaela Rocha Pinto¹, Silvana Mattedi², Martin Aznar¹
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²*Department of Chemical Engineering, Federal University of Bahia, Brazil*
- P-65 **Aggregation behavior of [C₁₂mim][OAc] surface active ionic liquid and dynamic interfacial tension in systems with crude oil and water/brine**
Iago Rodríguez-Palmeiro, Iria Rodríguez-Escontrela, Oscar Rodríguez, Alberto Arce, Ana Soto
University of Santiago de Compostela, Spain
- P-66 **Characterisation of mixtures of the ionic liquid 1-ethyl-3-methylimidazolium acetate with light alkanols**
María C. Castro, Héctor Rodríguez, Alberto Arce, Ana Soto
Department of Chemical Engineering, University of Santiago de Compostela, Spain
- P-67 **Molecular design of carbon dioxide physical absorption solvents**
Francisco Sánchez, Selva Pereda, Esteban A. Brignole
PLAPIQUI - UNS CONICET, Argentina
- P-68 **Influence of water concentration in the viscosities and densities of cellulose dissolving ionic liquids**
Cristina Jiménez de la Parra, Johnny R. Zambrano, M^a Dolores Bermejo, Ángel Martín, M^a José Cocero, José J. Segovia
University of Valladolid, Spain
- P-69 **Solubility of polycyclic aromatic hydrocarbons in ionic liquids**
Anabela. J. L. Costa, José N. Canongia Lopes, José M. S. S. Esperança, Luís Paulo N. Rebelo
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- P-70 **Ionic liquids as co-solvents for polyaromatic hydrocarbons solubilisation in water**
Fátima Moscoso, Ana B. Pereiro, José N. Canongia Lopes, José M. S. S. Esperança, Luís Paulo N. Rebelo
Instituto de Tecnologia Química e Biológica, Universidade Nova de Lisboa, Portugal
- P-71 **Palladium(II) hexafluoroacetylacetonate [Pd(hfac)₂] impregnation on silica [SiO₂] using supercritical carbon dioxide [CO₂]**
Alexander Junges¹, Bruna de Araujo Queiroz¹, Cláudio Dariva¹, Sílvia Maria Egues Dariva¹, Juliana Faccin de Conto Borges¹, Gustavo Borges, Eunice Valduga², Elton Franceschi¹
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²*Departamento de Engenharia de Alimentos, Universidade Regional Integrada do Alto Uruguai e das Missões, Brazil*

- P-72 **Silica (SiO₂) microparticles precipitation using supercritical carbon dioxide (CO₂) as anti solvent by SEDS technique**
Alexander Junges¹, Cláudio Dariva¹, Gustavo R. Borges¹, Sílvia M. Egues Dariva¹, Eunice Valduga², Marcos Hiroiuqui Kunita³, Elton Franceschi¹
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²*Departamento de Engenharia de Alimentos, Universidade Regional Integrada do Alto Uruguai e das Missões, Brazil*
³*Departamento de Química, Universidade Estadual de Maringá, Brazil*
- P-73 **Developing supercritical antisolvent fractionation to obtain bioactives from *Crocus sativus* corms**
Viviana Hinojosa¹, Leidy J. Jiménez-Coqueco¹, A. González-Coloma², Omar Santana-Méridas³, José S. Urieta¹, Juan I. Pardo¹, Ana M. Mainar¹
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³*Departamento de Cultivos Herbáceos / Centro Agrario de Albadalejito, Cuenca, Spain*
- P-74 **Supercritical fractionation of antioxidants from algerian *Opuntia ficus-indica* (L.) Mill. seeds**
Souad Khaled¹, Khodir Madani¹, José S. Urieta², Ana M. Mainar¹
¹*Laboratory of Biomathematics, Biochemistry, biophysics and Scientometrics, University of Bejaia, Algeria*
²*Aragon Institute for Engineering Research (I3A) / Univ. de Zaragoza, Spain*
- P-75 **Equation of state predictions of the separation of acid gases from natural gas using an ionic liquid**
M.T. Mota-Martinez, Maaïke C. Kroon, Cor J. Peters
Eindhoven University of Technology, The Netherlands
- P-76 **Solubility of caffeine and ferulic acid in ethyl lactate + water mixtures**
David Villanueva Bermejo¹, Tiziana Fornari¹ and Roumiana P. Stateva²
¹*Instituto de Investigación en Ciencias de la Alimentación CIAL (CSIC-UAM), Spain*
²*Institute of Chemical Engineering, Bulgarian Academy of Sciences, Bulgaria*
- P-77 **Rheological behaviour of the ionic liquid [N_{444H}][NTf₂]**
Angela Lamas and Teófilo Graber
Universidad de Antofagasta, Chile
- P-78 **Modeling the vapor-liquid equilibria and water activities of aqueous ionic liquids**
Mariana B. Oliveira¹, Emanuel Crespo¹, Felix Llovel², Lourdes F. Vega², João A. P. Coutinho¹
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TOPIC 4. Energy. Gas and oil. Petrochemicals. Environment and sustainability

- P-79 **Equilibrium isotherm of isolan red biosorption onto non-living leaves of *Posidonia oceanica***
*Juan F. Ortuño**, *M^a Isabel Aguilar*, *Víctor F. Meseguer*, *José Sáez*,
Mercedes Lloréns, *Ana Belén Pérez-Marín* and *Ana Lorena Picón*
Universidad de Murcia, Spain
- P-80 **Biosorption kinetic of methylene blue on brewery waste**
Víctor F. Meseguer, *Juan F. Ortuño**, *M^a Isabel Aguilar*, *Ana Belén Pérez-*
Marín, *José Sáez*, *Mercedes Lloréns*, and *Matilde Sánchez-Peña*
Universidad de Murcia, Spain
- P-81 **Using the F-SAC model to predict the behavior of ethanol-water-glycerol mixtures for the application in a extractive distillation process**
Henrique Mezzomo and *Rafael de Pelegrini Soares*
Universidade Federal do Rio Grande do Sul, Brazil
- P-82 **Analysis and implementation of different methods for characterization of heavy fractions in reservoir fluids**
Martin Cismondi¹, *Nicolas Heredia¹*, *Rafael Pereira do Carmo³*, *Papa Matar Ndiaye²*, *Frederico W. Tavares²*
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²*Escola de Química – Universidade Federal do Rio de Janeiro, Brazil.*
³*Programa de Engenharia Química/COPPE – Universidade Federal do Rio de Janeiro, Brazil*
- P-83 **Dehydration of bioethanol at the pilot plant scale using naphthas as entrainers**
Jorge García-Cano, *Vicente Gomis*, *María Dolores Saquete*, *Alicia Font.*
Department of Chemical Engineering, University of Alicante, Spain
- P-84 **Dehydration of biobutanol using hexane and cyclohexane as entrainers: simulation and pilot plant scale experiment**
Jorge Garcia-Cano, *Vicente Gomis*, *Maria Dolores Saquete*, *Alicia Font*,
Rosa Diaz.
Department of Chemical Engineering, University of Alicante, Spain

TOPIC 5. Biomolecules and Biotechnology

- P-85 **Striving against α -amylase deactivation in the presence of ionic liquids**
Diana Ruivo¹, *Marita A. Cardoso³*, *Verónica Z. Bermudez³*, *Francisco J. Deive^{1,2}*, *Ana Rodríguez^{1,2}*, *Luís Paulo N. Rebelo¹*, *José M. S. S. Esperança¹*
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P-86 On the hunt for truly biocompatible ionic liquids for lipase-catalyzed reactions

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P-87 Use of atomic force microscopy and light scattering for the characterization of the structure of polymeric systems

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P-88 Antiproliferative activity of supercritical plant extracts on pancreatic cancer cell line

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TOPIC 6. Product and Process Design. Databases and Software

P-89 Surface tension of three families of alcohols. Selection of data and correlation

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P-90 Fractionation of fatty esters and acylglycerols by liquid CO₂

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