

ORAL PRESENTATIONS

MONDAY, 22 October	
Session 1	
18:50 – 19:05	Molecular dynamics simulations of electrolyte solutions confined by calcite nanopores <u>Mirella Simoes Santos</u> , Marcelo Castier and Ioannis G. Economou <i>Chemical Engineering Program, Texas A&M University at Qatar, Qatar.</i>
19:05 – 19:20	Human islet amyloid polypeptide: Identifying early-stage aggregation mechanisms through molecular simulation <u>Ashley Guo</u> and Juan de Pablo <i>Institute for Molecular Engineering, The University of Chicago, USA.</i>
19:20 – 19:35	Towards a solvent screening tool for CO ₂ capture applications: Predicting the phase behaviour of CO ₂ -amine blends from single amine mixtures <u>Luís M. C. Pereira</u> and Lourdes F. Vega <i>Gas Research Center and Chemical Engineering Department, The Petroleum Institute, Khalifa University of Science and Technology, Abu Dhabi, UAE.</i>
19:35 – 19:50	Carbon dioxide capture by alkanolamine (MEA, DEA, MDEA) in deep eutectic solvent medium (choline chloride: ethylene glycol) Mohammed-Ridha Mahi ^{1,2} , Ilham Mokbel ^{1,3} , <u>Latifa Negadi</u> ^{2,4} and Jacques Jose ¹ ¹ <i>Laboratoire Multimatériaux et Interfaces, Université Claude Bernard, Villeurbanne, France.</i> ² <i>LATA2M, Laboratoire de Thermodynamique Appliquée et Modélisation Moléculaire, University of Tlemcen, Algeria.</i> ³ <i>Université de Lyon, UJM, Saint Etienne, France.</i> ⁴ <i>Thermodynamics Research Unit, School of Engineering, University of KwaZulu-Natal, Howard College Campus, Durban, South Africa.</i>
TUESDAY, 23 October	
Session 2	
10:40 – 10:55	Electrical double-layer and wettability of brine, calcite, and oil interfaces <u>Nathalia S. V. Barbosa</u> ¹ , Pedro H. R. Alijó ¹ , Eduardo R. A. Lima ¹ and Frederico W. Tavares ^{2,3} ¹ <i>Institute of Chemistry, Rio de Janeiro State University, Brazil.</i> ² <i>School of Chemistry, Federal University of Rio de Janeiro, Brazil.</i> ³ <i>Chemical Engineering Program, Alberto Luiz Coimbra Institute for Graduate Studies, Federal University of Rio de Janeiro, Brazil.</i>
10:55 – 11:10	Near-infrared spectroscopy for detection of asphaltene precipitation onset in model systems induced by CO ₂ <u>Denisson Santos</u> ¹ , Arley A. Cruz ¹ , Monique Amaral ¹ , Gustavo R. Borges ¹ , Elton Franceschi ¹ , João A. P. Coutinho ² , Julio Palácio ³ and Cláudio Dariva ¹ ¹ <i>NUESC/ITP, Núcleo de Estudos em Sistemas Coloidais, PEP/PBI/UNIT, Universidade Tiradentes, Aracaju, Brazil.</i> ² <i>CICECO, Department of Chemistry, University of Aveiro, Portugal.</i> ³ <i>ISPG/PETROGAL BRASIL, Rio de Janeiro, Brasil.</i>
11:10 – 11:25	(to be confirmed)
11:25 – 11:40	(to be confirmed)

WEDNESDAY, 24 October

Session 3

10:20 – 10:35	<p>Modelling the solvation of non self-associating species: An extensive investigation in the SAFT framework <u>Jamie Cripwell</u> and Andries Burger <i>Department of Process Engineering, Stellenbosch University, Western Cape, South Africa</i></p>
10:35 – 10:50	<p>Experimental data and thermodynamic modeling of physicochemical properties for the design of supercritical hydrogenation reactors <u>Pablo Hegel</u>¹, Natalia Cotabarren¹, Esteban A. Brignole¹ and Selva Pereda^{1,2} ¹ PLAPIQUI – DIQ, Universidad Nacional del Sur (UNS) – CONICET, Bahía Blanca, Argentina. ² Thermodynamics Research Unit, School of Engineering, University of KwaZulu-Natal, Howard College Campus, South Africa.</p>

Session 4

17:00 – 17:15	<p>Phase behavior of ternary system (carbon dioxide + ω-pentadecalactone + dichloromethane) at high pressures Evertan A. Rebelatto¹, João P. Bender², J. Vladimir de Oliveira¹ and <u>Marcelo Lanza</u>¹ ¹ Department of Chemical Engineering and Food Engineering, Federal University of Santa Catarina, Florianópolis, SC, Brazil. ² Federal University of Fronteira Sul, Chapecó, SC, Brazil.</p>
17:15 – 17:30	<p>Solubility of p-coumaric acid and physico-chemical properties in distillable protic ionic liquids media <u>Silvana Mattedi</u>¹, Fabricio Ferrarini², Rafael Soares², Antonio Patti³ and Douglas MacFarlane³ ¹ Graduate Program in Chemical Engineering, Federal University of Bahia, Brazil. ² Graduate Program in Chemical Engineering, Federal University of R. G. do Sul, Brazil. ³ School of Chemistry, Monash University, Australia.</p>
17:30 – 17:45	<p>Experimental data of solid-fluid phase equilibria for the system scCO₂ (1) + CBD (2) <u>Daniel Ribeiro Grijó</u>¹, Gryele Karen Piva¹, Vladimir Ferreira Cabral¹ and Lúcio Cardozo-Filho^{1,2} ¹ Department of Chemical Engineering/Graduate Program in Chemical Engineering, Universidade Estadual de Maringá, Brazil. ² Center for Research, Centro Universitário da Fundação de Ensino Octávio Bastos, Brazil.</p>
17:45 – 18:00	<p>Recovery of flavonoids using novel biodegradable choline amino acids ionic liquids based ATPS Elena Gómez, Patricia F. Requejo and <u>Eugénia A. Macedo</u> <i>Associate Laboratory of Separation and Reaction Engineering – Laboratory of Catalysis and Materials (LSRE-LCM), Department of Chemical Engineering, Faculty of Engineering, University of Porto, Portugal.</i></p>

THURSDAY, 25 October

Session 5

11:20 – 11:35	<p>Procedure for the correlation of normal appearance VLE data where the classical models dramatically fail with no apparent reason <u>Antonio Marcilla</u>, Juan A. Reyes-Labarta and María del Mar Olaya <i>Department of Chemical Engineering, University of Alicante, Spain.</i></p>
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11:35 – 11:50	<p>Computation and analysis of binary multiphase isochores Matías J. Molina¹, <u>Sabrina B. Rodriguez-Reartes</u>^{1,2} and Marcelo S. Zabaloy^{1,2} ¹ <i>Planta Piloto de Ingeniería Química – PLAPIQUI (UNS-CONICET), Argentina.</i> ² <i>Departamento de Ingeniería Química, Universidad Nacional del Sur (UNS), Argentina.</i></p>
11:50 – 12:05	<p>Modeling strategies for the phase behavior simulation of amazonian fats and oils <u>Ericsem Pereira</u>, Antonio José de Almeida Meirelles and Guilherme José Maximo <i>Laboratory of Extraction, Applied Thermodynamics and Equilibrium, School of Food Engineering, University of Campinas, Brazil.</i></p>
12:05 – 12:20	<p>Application of the associative and polar SAFT-VR Mie molecular models to acetone and their mixtures <u>José Matías Garrido</u>¹ and Ilya Polishuk² ¹ <i>Departamento de Ingeniería Química, Universidad de Concepción, Chile.</i> ² <i>Department of Chemical Engineering & Biotechnology, Ariel University, Israel.</i></p>