ORAL PRESENTATIONS

MONDAY, 22 October	
Session 1	
18:50 – 19:05	Molecular dynamics simulations of electrolyte solutions confined by calcite nanopores Mirella Simoes Santos, Marcelo Castier and Ioannis G. Economou *Chemical Engineering Program, Texas A&M University at Qatar, Qatar.*
19:05 – 19:20	Human islet amyloid polypeptide: Identifying early-stage aggregation mechanisms through molecular simulation Ashley Guo and Juan de Pablo *Institute for Molecular Engineering, The University of Chicago, USA.*
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 Luís M. C. Pereira and Lourdes F. Vega *Gas Research Center and Chemical Engineering Department, The Petroleum Institute, Khalifa University of Science and Technology, Abu Dhabi, UAE.*
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], Latifa Negadi[2,4] and Jacques Jose[1] *[1] Laboratoire Multimatériaux et Interfaces, Université Claude Bernard, Villeurbanne, France.* *[2] LATA2M, Laboratoire de Thermodynamique Appliquée et Modélisation Moléculaire, University of Tlemcen, Algeria.* *[3] Université de Lyon, UJM, Saint Etienne, France.* *[4] Thermodynamics Research Unit, School of Engineering, University of KwaZulu-Natal, Howard College Campus, Durban, South Africa.*
TUESDAY, 23 October	
Session 2	
10:40 – 10:55	Electrical double-layer and wettability of brine, calcite, and oil interfaces Nathalia S. V. Barbosa[1], Pedro H. R. Alijó[1], Eduardo R. A. Lima[1] and Frederico W. Tavares[2,3] *[1] Institute of Chemistry, Rio de Janeiro State University, Brazil.* *[2] School of Chemistry, Federal University of Rio de Janeiro, Brazil.* *[3] Chemical Engineering Program, Alberto Luiz Coimbra Institute for Graduate Studies, Federal University of Rio de Janeiro, Brazil.*
10:55 – 11:10	Near-infrared spectroscopy for detection of asphaltene precipitation onset in model systems induced by CO_2 Denisson Santos[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] NUESC/ITP, Núcleo de Estudos em Sistemas Coloidais, PEP/PBI/UNIT, Universidade Tiradentes, Aracaju, Brazil.* *[2] CICECO, Department of Chemistry, University of Aveiro, Portugal.* *[3] ISPG/PETROGAL BRASIL, Rio de Janeiro, Brasil.*

11:10 – 11:25	Effect of carbon dioxide on the viscosity of undersaturated hydrocarbon mixtures at high pressures Luciana L. de Pinho Rolemberg de Andrade and Krishnaswamy Rajagopal *Escola de Química, Laboratório de Termodinâmica e Cinética Aplicada (LATCA), Universidade Federal do Rio de Janeiro, Brazil.*
11:25 – 11:40	A comparative study of CPA and PC-SAFT equations of state to calculate the asphaltene onset pressure and phase envelope Fabio P. Nascimento[1], Gloria M.N. Costa[1] and Silvio A.B. Vieira de Melo[1,2] *[1] Programa de Pós-Graduação em Engenharia Industrial, Escola Politécnica, Universidade Federal da Bahia, Brasil.* *[2] Centro Interdisciplinar em Energia e Ambiente, Campus Universitário da Federação/Ondina, Universidade Federal da Bahia, Brasil.*
WEDNESDAY, 24 October	
Session 3	
10:20 – 10:35	Application of the associative and polar SAFT-VR Mie molecular models to acetone and their mixtures José Matías Garrido[1] and Ilya Polishuk[2] *[1] Departmento de Ingeniería Química, Universidad de Concepción, Chile.* *[2] Department of Chemical Engineering & Biotechnology, Ariel University, Israel.*
10:35 – 10:50	Experimental data and thermodynamic modeling of physicochemical properties for the design of supercritical hydrogenation reactors Pablo Hegel[1], Natalia Cotabarren[1], Esteban A. Brignole[1] 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.*
Session 4	
17:00 – 17:15	Phase behavior of ternary system (carbon dioxide + ω-pentadecalactone + dichloromethane) at high pressures Evertan A. Rebelatto[1], João P. Bender[2], J. Vladimir de Oliveira[1] and Marcelo Lanza[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.*
17:15 – 17:30	Solubility of p-coumaric acid and physico-chemical properties in distillable protic ionic liquids media Silvana Mattedi[1], Fabricio Ferrarini[2], Rafael Soares[2], Antonio Patti[3] and Douglas MacFarlane[3] *[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.*
17:30 – 17:45	Solubility of bioinsecticides in supercritical CO_2. Experimental measurement and modeling with the GC-EOS Nicolás Gañán[1], Hernán Mazzei[2], Leonardo Ortega[2] and Alfonsina Andreatta[3] *[1] IPQA (UNC-CONICET), Universidad Nacional de Córdoba, Argentina.* *[2] ICTA (FCEFYN-UNC), Universidad Nacional de Córdoba, Argentina.* *[3] Universidad Tecnológica Nacional (UTN-Regional San Francisco), Argentina.*

17:45 – 18:00	Recovery of flavonoids using novel biodegradable choline amino acids ionic liquids based ATPS Elena Gómez, Patricia F. Requejo and Eugénia A. Macedo *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.*
THURSDAY, 25 October	
Session 5	
11:20 – 11:35	Procedure for the correlation of normal appearance VLE data where the classical models dramatically fail with no apparent reason Antonio Marcilla, Juan A. Reyes-Labarta and María del Mar Olaya *Department of Chemical Engineering, University of Alicante, Spain.*
11:35 – 11:50	Computation and analysis of binary multiphase isochores Matías J. Molina[1], Sabrina B. Rodriguez-Reartes[1,2] and Marcelo S. Zabaloy[1,2] *[1] Planta Piloto de Ingeniería Química – PLAPIQUI (UNS-CONICET), Argentina.* *[2] Departamento de Ingeniería Química, Universidad Nacional del Sur (UNS), Argentina.*
11:50 – 12:05	Modeling strategies for the phase behavior simulation of amazonian fats and oils Ericsem Pereira, Antonio José de Almeida Meirelles and Guilherme José Maximo *Laboratory of Extraction, Applied Thermodynamics and Equilibrium, School of Food Engineering, University of Campinas, Brazil.*