Poster Sessions

Nr Soum.	Author	Poster title
		TUESDAY 6 JUNE - SESSION 1
21	Hermida-Merino	Structural characterization of graphene IoNanofluids designed for gas absorption processes
94	Wilhelmsen	Phase diagrams for heterogeneous structures in pores for mitigation of corrosion under insulated pipes
103	Singh	Discovery of novel high-pressure ice polymorphs in diamond confinement
263	Gil-Villegas	Computer simulations of quantum effects on the surface tension of liquids
31	Langenbach	Static and dynamic properties of interfaces in Lennard-Jones systems
41	Haghbakhsh	A novel global model for the estimation of surface tensions of deep eutectic solvents
184	Ji	Modelling interfacial properties with Spot-DGT-PC-SAFT for binary mixtures including ionic liquid-CO2 system
249	Blas	Vapour-liquid phase equilibria and interfacial properties of tetrahydrofuran + methane from the combination of experiments, simulation, and theory
336	Lins	New correlations to model the CO2-aqueous phase interfacial tension at the Brazilian pre-salt reservoir conditions
354	El Kadiri	Water-ater-aromatic inteface: some insights from molecular simulation
96	Sun	Molecular dynamics simulation of heat and mass transfer for liquid argon flow in a 2D channel
102	Moultos	Thermophysical properties of aqueous reline and ethaline solutions from molecular dynamics simulation
149	Bernet	Microscopic structure and interfacial properties of confined Mie fluids using classical DFT
379	AlJabri	The effect of changing the molecular structure of the surfactant on the dissolution of lamellar phases
305	Mougin	Confined systems approcheas in classical thermodynamics: a benchmark study
95	Wieckowski	Eutatic phase change materials - measurements and thermodynamic modeling
117	Karakatsani	Modeling study of amine- containing complex systems
277	Klimosek	Phase equilibria relevant for catalytic olefin polymerization in fludized bed reactors
151	Petrov	Features of intermolecular interactions in binary solvents – azeotropes
198	Fakhurtdinova	Excess volume as a parameter for estimation the contributions of intermolecular interactions

9	Kulkarni	A force field for poly (oxymethylene) dimethy ethers (OMEn)
65	Stephan	A database for molecular models for the simulation of thermodynamic properties of fluids
211	Jimenez Serratos	Small-angle neutron scaterring calculated from coarse-grained molecular dynamics simulations
270	Fayaz Torshizi	Coarse-grained molecular dynamics study of the self-assembly of triblock bolaamphiphiles with SAFT-γ Mie CG forcefield
365	Khennache	Thermophysical properties prediction: towards a unified approach
353	Yan	Measurement and modeling of high-pressure diffusion coefficients of methane in pure hydrocarbons and reservoir fluids
163	Mahamoudou	State of the art of thermodynamic analysis of falling film in absorber
206	Akhmadiyarov	Study of the influence of thermobaric conditions on the density and rheological properties of crude oil from Ashalchinskoye field in the presence of supercritical
335	Lins	Modeling viscosity in systems containing brine, formation water and CO2 saturated brine at high pressure and temperature
330	Munoz-Rujas	Density, viscosity and refractive index of binary mixture dibutyl ether + 2-propanol: experimental data and PC-saft equation of state modeling
382	van den Bruinhorst	Determination of the enthalpy of fusion of choline chloride using dissolution and titration calorimetry
362	Moreau	Speeds of sound and derived properties of (C3H8 + CO) mixtures
173	Brocus	Correlating solubility and kinematic viscosity data for Daniel plots
85	e Azevedo Medeiro	State-function based flash specifications for open systems in the absence or presence of chemical reactions
210	Qu	Efficient phase equilibrium computations using learning algorithms
190	Hoceini	New approach for improving the representation of phase equilibrium in the presence of solid phases:
191	Fleitmann	What to measure for optimal predictions of process performance? Optimal design of phase equilibria
299	Spatolisano	Impact of thermodynamic modeling in helium recovery and upgrading processes
		WEDNESDAY 7 JUNE - SESSION 2
182	Ricci	Effects of CO2 sorption on structure and local dynamics of atactic polystyrene melts from molecular simulations
276	Krajakova	Two-phase and three-phase equilibira important for catatlytic ethylene polymerization in liquid
220	Creton	Prediction of the quantity of a penetrant sorbed into a polymer matrix using machine learning
203	De Angelis	Modeling sorption of CO2 in polyelectrolites with the pePC-SAFT equation of state: the case of CO2
100	Esper	Experimental determination of phase equilibrium properties of aldhydes, Ketones and formates
135	El Ahmar	Excess molar volumes and enthalpies of binary mixtures containing furan at temperatures up to 383.15 K and pressure up to 2.1 Mpa
227	Fele-Zilnik	Hydrogen solubility in guaiacol, levulinic acid+water and 5-hydroxymethylfurtural + water
287	Abranches	Understanding the formation of deep eutectic solvents: betaine as a universal hydrogen bond acceptor

361	Rakipov	Thermochemistry of dissolution, solvation and hydrogen bonding of linear and cyclic esters in solvents
331	Munoz-Rujas	Experimental data and modeling of thermophysical properties of mixtures of (Oxygenated additives + alcohol)
284	Arkhipin	Thermodynamic model of the water – nitric acid – lanthanum nitrate –di-(2-ethylhexyl) phosphoric acid
251	Georgiopoulou	Comparative study of conventional and alternative extraction techniques of high added value compounds from Chlorella Vulgaris
369	Soto	Enhanced dissolution kinetics of lidocaine in simulated biological fluids via eutectic formation with polyethylene glycols
346	Passarello	Development of a fully analytical equation of state using realistic interaction potentials. Simple fluids : application to rare gases.
377	Kud	Improvements for a fully consistent description of the new semi-empirical vapor density model
59	Mejia	Phasepy: a Python based framework for fluid phase equilibria computation
386	Fleck	Transferable anisotropic Mie-potential force field for amines and non n-alcohols
264	Bauer	Transferable anisotropic united-atom Mie (TAMie) force field: transport properties from equilibrium molecular dynamics simulations
35	Graczova	VLE description of ternary systems containing imidazolium ionic liquid
46	Zhang	Modelling phase behavior and thermal-properties of ammonia-water with CPA
356	Tasios	A group contribution volume translated equation of state
166	Walker	A new predictive group-contribution ideal-heat-capacity model, and its influence on second-derivative properties calculated using a free-energy equation of state
200	Petropoulou	A group-contribution approach for the modelling of industrially important associating mixtures
266	Di Pietro	Prediction of phase equilibria of mixtures containing ionic liquids or deep eutectic solvents using COSMO based models
8	Kulkarni	Multicriteria optimisation of molecular models of water using the reduced units method
177	Villazon Leon	Development of an improved group contribution model for the prediction of critical properties of
189	Miyazaki	Prediction of activity coefficient at infinite dilution (γ^{∞}) and vapor-liquid equilibira (VLE) of binary systemes by COSMO-SAC
223	Kohns	Molecular simulation study of the relative permittivity of pure fluids and mixtures
261	Wieckowski	Propils: an extensive ionic liquids properties databank along with a set of versatile empirical models for property estimation
383	Tran	Predicting octanol/water partition coefficients from molecular structure
308	Eusebio	Lyotropic ionic liquid crystal gel: structure-properties relations
396	Gantzer	NEW TOOL FOR THE COMPARISON OF MOLECULAR STRUCTURES GENERATIONS
375	Roa Pinto	Short-range ion-solvent and ion-ion interactions within the framework of the primitive equations of state
250	Maliutin	Thermodynamic model of the UO22+, Ca2+, H+ // NO3-, H2O system
296	Albahrani	Developing a group contribution method for the prediction of gas/vapor solubility coefficient in glassy polymers

325	Hayer	Prediction of Henry's law constants by matrix Completion
338	Atiq	Multiscale modelling of gas sorption in semicrystalline polymers
341	Asensio-Delgado	Ionic liquids as entrainers of fluorinated refrigerant gases: from vapor-liquid equilibrium to separation
140	Dumas	Evaluation of some physical properties of (U,Pu)O2 fuel by thermodynamic calculations
		THURSDAY 8 JUNE - SESSION 3
28	Tsochantaris	Application and evaluation of CPA and PC-SAFT on water for different sets of parameters
84	Yan	Comparison of engineering models and their volume-translated versions in describing high-pressure
105	Klajmon	PC-saft parameterization of pharmaceuticals based on more than experimental solubility data
332	Borrmann	Prediction of water sorption in amorphous pharmaceuticals
193	Valsecchi	Modelling the thermodynamic properties of aqueous mixtures of poly (etylene glycol) through the SAFT-γ Mie equation of state
238	Chapman	Self-assembly and phase behavior of hyperbranched copolymers
4	Xu	SAFT model in industrial scale dynamic simulation applications
83	Ramirez-Velez	Which associating compounds absolutely need an association term to be correctly modeled with a SAFT-type equation of state?
66	Stephan	Comprehensive evaluation of equations of state of the Lennard-Jones fluid
142	Liang	Critical point of associating fluids from the CPA EOS
351	Yew	OpenSAFT: an extensible Julia implementation of SAFT-type equations of state
74	Schwarz	Accurate thermodynamic description of quadrupolar molecules and their mixtures in SAFT-VR Mie
129	Cripwell	Modelling polarity and solvation in multicomponent systems using a polar SAFT variant
366	Khennache	Revisiting the Lennard-Jones Chain fluid properties
36	Nelson	Liquid-vapor phase equilibrium of a simple liquid confined in a random porous media: second-order
136	El Ahmar	Density and thermal properties of CCTS fluid systems
147	Secuianu	Phase equilibria in systems of interest for CCS
272	Tuma	High-pressure density data of binary (carbon dioxide + oxygen) mixtures for the development of
201	Williams-Wynn	Assessing the performance of amine blends for post-combustion CO2 capture
202	de Angelis	Modeling the competitive absorption of H2S and CO2 in aqueous methyldiethanolamine (MDEA) solutions
294	De Guido	Application of phase equilibria analysis in the presence of solid carbon dioxide to the sweetening of natural gas
179	Abraham Diego	Comparison of EoS for the simulation of extraction processes using supercritical fluids

90	Delgado	CO2 absorption into aqueous solution of PZ and MDEA/PZ: physical properties and equilibrium review
360	Neto	Prediction of thermophysical properties for CO2 and CO2 rich mixtures from CPA EoS
187	Gomez Costas	Thermal analysis of binary mixtures of NTF2- and TFO- ionic liquids
268	Di Pietro	Determination of thermodynamic properties of Ether-Functionalized Tetraalkylammonium and
381	Vaz	Absorption of gaseous alkanes and alkenes by ionic liquids containing phosphorous
262	Queiros	Study of thermophysical properties of new ionic liquid based mixtures (1-ethyl-3-methylimidazolium ethylsuflate/water) for absorption refrigeration
358	Graczova	VLE description of ternary systems containing imidazolium ionic liquids
367	Soto	Design of formulations based on ionic liquids for low-tension oil recovery processes: Phase behavior tests
		FRIDAY 9 JUNE - SESSION 4
10	Ferrando	Modeling phase equilibrium of hydrogen and natural gas in brines: application to storage in salt caverns
33	Simonin	Organic electrolyte solutions: deviations from ideality described within the binding mean spherical approximation
127	Sum	A new approach for correlating the solution properties of strong electrolyte systems
180	Olsen	Testing the Limits of an Equation of State based on the Primitive Model for Electrolytes: the System
216	Rezazadeh	Modeling and experimental study of the electrolyte system of Disodium Terephthalate, Water,
292	Kournopoulos	Molecular theory of the static dielectric constant of a dipolar fluid
376	Yang	The (water + alcohol + alkali halide) mixed-solvent electrolyte systems: data status and consistency analysis
395	Neumaier	Modeling the dielectric constant of mixed solvents based on perturbation theory
34	Graczova	VLE Measurement of binary systems containing ionic liquid
172	Kijevcanin	Experimental measurements of thermophysical properties and theoretical quantum chemical calculations
78	Marliere	Methodologies for thermodynamic properties characterization in microfluidic systems
69	Goutaudier	The effect of antioxidant additives on physicochemical properties of a surrogate gasoline
207	Akhmadiyarov	High pressure high temperature density of benzene-cyclohexane mixtures
285	Lorenzo	The understanding of the thermophysical behavior of biodiesel-based synthetic fuels using experimental
363	Moreau	Viscosities and densities of alcohols at high pressures
75	Schwarz	Phase behaviour of the quaternary water + (ethanol + 2-propanol) + isooctane system
368	Soto	Preparation and characterization of eutectics for application in enhanced oil recovery
371	Paricaud	Modelling of the thermophysical properties of a-tochopherol+ethanol+n-pentane and a-tocopherol

159	Nelson	Purification of nitrogen trifluoride via physical absorption
171	Radovic	High pressure densities of ethylene glycol and caffeine mixtures
148	Secuianu	Phase equilibria and densities of carbon dioxide (1) + n-pentane (2)
281	de Hemptinne	Calculation of LLE in electrolyte solutions
378	Gaganis	Bridging the gap between stability and phase split calculations
62	Stoyanova	Thermodynamic entropy production for characterizing regional climate variability and natural
253	Georgiopoulou	Development and economic evaluation of a recycling process for Tetra-Pak®packaging
326	Fermeglia	Carbon Capture and Sequestration process sustainability prediction: process simulation as a base for
344	Braccio	Cold and electricity cogeneration from a low temperature heat source through an absorption process
348	Lhermet	Experimental and numerical study of an organic rankine cycle using NOVEC649, HFE7000, HFE7100 and
343	Baiguini	Discrete model for the behavior of cryogenic fluids in small-scale tanks
43	Haghbakhsh	An experimental investigation on the viscosities of the DES (1 choline chloride + 4 phenol) in mixtures with water
146	Pineiro	Triphasic coexistence temperature of HFC hydrates determined using molecular dynamics
205	Nieto-Draghi	Salinity change of critical micelle concentration of anionic surfactants: direct comparison of experiments
329	Lopes	Modeling hard cylinders: from liquid crystals to industrial relevant fluids
45	Moultos	Inclusion complexation of organic micropollutants with β-Cyclodextrin
1	Popovic	Thermodynamic properties of microorganisms: Determination and analysis of enthalpy, entropy, and Gibbs free energy of biomass and microorganisms
176	Pereiro	Disclosing the interactions of flurorinated ionic liquids with therapeutic proteins
214	Dardavila	Recovery of bioactive compounds from microalgae using novel solvents
380	Sadeghi	Phase equilibria of amino acid molecules forming solid solutions