

25th European Symposium on Applied Thermodynamics

**June 24-27, 2011
Saint Petersburg, Russia**



ESAT 2011

BOOK OF ABSTRACTS

**Saint Petersburg State University
Institute of Macromolecular Compounds, Russian Academy of Sciences
The Mendeleev Russian Chemical Society**

**CD ROM
Included**

CONTENTS

Committees	V
History of ESAT Meetings	VI
Preface	VII
Conference Timetable	IX
Scientific Program	XV
Abstracts	1
Oral Program	3
Poster Session I	157
Poster Session II	293
Author Index	425
List of Participants	435

	Session 4: Surfactants, Polymers and Bio- Related Systems (Ceremony Hall, main building) Chair: E. Macedo, S. Enders	Session 5: Molecular Thermodynamic modeling, theory and computer simulation (Peter's Hall, main building) Chair: K. Aim, L. Vega	Session 6: Interfacial phenomena (Chemistry Center building) Chair: A. Rusanov, M. Anisimov
15.30 – 15.50	J. Kosek (p. 53)	F. Llovell (p. 67)	D.V. Tatyanyenko (p. 79)
15.50 – 16.10	P. Schrader (p. 55)	P. Paricaud (p. 69)	F. Hodaj (p. 81)
16.10 – 16.30	S. Wille (p. 57)	S. Deublein (p. 71)	J.K. Singh (p. 82)
16.30 – 16.50	J.P. O'Connell (p. 59)	J.R. Elliott (p. 72)	M.R. Dehghani (p. 83)
16.50 – 17.10	F.L. Mota (p. 60)	I. Nezbeda (p. 74)	M. Horsch (p. 85)
17.10 – 17.30	S. Hempel (p. 62)	S. Sazhin (p. 75)	M. Kosmulski (p. 87)
17.30 – 19.30	Poster Session 1 (p. 157)		
19.30 – 21.00	Dinner		
21.00 – 22.30	City tour		

SUNDAY, 26.06.2011

Plenary session (Ceremony Hall, main building) Chair: N. Smirnova, J.-N. Jaubert			
09.00 – 09.30	L.F. Vega (p. 91)		
09.30 – 10.15	I. Smirnova (p. 93)		
10.15 – 10.45	M. Francisco (p. 94)		
10.45 – 11.15	Coffee break		
	Session 7: Surfactants, Polymers and Bio- Related Systems (Ceremony Hall, main building) Chair: G. Sadowski, I. Smirnova	Session 8: Phase Equilibria and Thermophysical Data: measurement, analysis and predictive tools (Peter's Hall, main building) Chair: M. Trusler, J. Gmehling	Session 9: Petroleum fluids (Chemistry Center building) Chair: E. Voutsas, E. Hendriks
11.15 – 11.35	V. Kocherbitov (p. 99)	E.A. Brignole (p. 113)	E. Neau (p. 125)
11.35 – 11.55	M.G. De Angelis (p. 101)	T.W. De Loos (p. 115)	M. Cismondi Duarte (p. 127)
11.55 – 12.15	J. Völkl (p. 103)	C. Secuianu (p. 116)	E. Skouras (p. 129)

<i>High-Pressure Densities of Ionic Liquids: Structure-Property Relations and New Measurements</i> <i>Regueira T., Lugo L., <u>Fernández J.</u></i>	49
--	----

SESSION 4: Surfactants, Polymers and Bio-Related Systems

Chair persons: E. Macedo, S. Enders

<i>Sorption equilibria and diffusion dynamics in semi-crystalline polymers</i> <i><u>Kosek J.</u>, <u>Hájová H.</u>, <u>Pokorný R.</u>, <u>Chmelař J.</u>, <u>Nistor A.</u></i>	53
--	----

<i>Phase Equilibria of Surfactant Containing Systems</i> <i><u>Schrader P.</u>, <u>Kulaguin – Chicaroux A.</u>, <u>Dorn U.</u>, <u>Enders S.</u></i>	55
---	----

<i>Modeling of Phase Equilibria in Microemulsion Systems Based on Partition Coefficients</i> <i><u>Wille S.</u>, <u>Sponsel E.</u>, <u>Mokrushina L.</u>, <u>Arlt W.</u></i>	57
---	----

<i>Applications of H-D Exchange Measurements for Protein Structure, Equilibria, and Kinetics</i> <i><u>O'Connell J.P.</u>, <u>Fernandez E.J.</u></i>	59
---	----

<i>Solubility of Drug-Like Molecules in Pure, Mixed and Supercritical Solvent Systems with the CPA EoS</i> <i><u>Mota F.L.</u>, <u>Queimada A.J.</u>, <u>Pinho S.P.</u>, <u>Macedo E.A.</u></i>	60
---	----

<i>Activity Coefficients and Structure of Water in Amino-Acid Solutions</i> <i><u>Hempel S.</u>, <u>Sadowski G.</u></i>	62
--	----

SESSION 5: Molecular Thermodynamic Modeling, Theory and Computer Simulation

Chair persons: K. Aim, L. Vega

<i>Thermodynamic modeling of cross-association systems with the soft-SAFT EoS</i> <i><u>Llovel F.</u>, <u>Vilaseca O.</u>, <u>Valente E.</u>, <u>Jung N.</u>, <u>Vega L.F.</u></i>	67
---	----

<i>Modeling of the dissociation conditions of salt hydrates and gas semiclathrate hydrates. Application to lithium bromide, hydrogen iodide hydrates, and mixed hydrates of gas + Tetra-n-butylammonium bromide</i> <i><u>Paricaud P.</u>, <u>Bouchafaa W.</u>, <u>Dalmazzone D.</u></i>	69
---	----

<i>Molecular Simulation of Aqueous Electrolyte Solutions – New Force Fields for Monovalent Anions and Cations</i> <i><u>Deublein S.</u>, <u>Reiser S.</u>, <u>Vrabec J.</u>, <u>Hasse H.</u></i>	71
---	----

<i>Accounting for Non-classical Critical Scaling with DMD/TPT in the Long Chain Limit</i> <i><u>Elliott J.R.</u>, <u>Ghobadi A.F.</u></i>	72
--	----

<i>A new concept for augmented van der Waals equations of state</i> <i><u>Nezbeda I.</u>, <u>Trokhymchuk A.</u>, <u>Melnyk R.</u></i>	74
--	----

Solubility of Drug-Like Molecules in Pure, Mixed and Supercritical Solvent Systems with the CPA EoS

Mota F.L.¹, Queimada A.J.¹, Pinho S.P.², Macedo E.A.¹

1 - Laboratory of Separation and Reaction Engineering (LSRE), Departamento de Engenharia Química, Faculdade de Engenharia, Universidade do Porto, Rua do Dr. Roberto Frias, 4200-465 Porto, Portugal

2 - Laboratory of Separation and Reaction Engineering (LSRE), Departamento de Tecnologia Química e Biológica, Instituto Politécnico de Bragança, Campus de Santa Apolónia, Apartado 1134, 530-857 Bragança, Portugal

fatima.mota@fe.up.pt

Most of the active pharmaceutical ingredients (API) are purified by crystallization being solubility a key property, and it also affects their efficacy, release, transport and absorption in the organism [1]. Although of extreme importance, data involving drug-like molecules are still scarce.

In recent years, efforts have been made towards the development of predictive tools to calculate phase behaviour of the API's. Thermodynamic models are important tools, and namely activity coefficient based models have been applied for that purpose. Still, these frequently cannot describe with the desired accuracy broad temperature and pressure ranges, various solvent compositions or multifunctional molecules. Despite the success of the cubic-plus-association (CPA) equation of state (EoS), only very recently it was applied to model the phase equilibria of drug-like molecules, explicitly accounting for the number and nature of associating sites [2-3].

In this work, the quality of the solubility estimates provided by the CPA EoS for a set of drug-like molecules in aqueous, pure and mixed organic solvents, and supercritical fluids will be presented, being the experimental data obtained from literature. Molecules containing different and/or multiple associating groups such as acetylsalicylic, adipic, ascorbic and stearic acids, acetamide, hydroquinone, ibuprofen and paracetamol were studied both in aqueous and organic systems in a wide temperature range [2-3]. In water, the solubility of acetanilide, bisphenol A, camphor, dibenzofuran, hexachlorobenzene, nicotinic and terephthalic acids, piperazine, sorbitol and vanillin were additionally predicted [2]. Mixed solvent systems of ascorbic, nicotinic, stearic and terephthalic acids, acetanilide, hexachlorobenzene, ibuprofen, paracetamol, sorbitol and vanillin in a wide range of compositions were also studied.

Generally, modelling results are within the experimental uncertainties using a single temperature independent binary interaction parameter. The good results found for some of the compounds in water are presented in Fig. 1(a), and for paracetamol in organic solvents in Fig. 1(b).

Besides the importance of the studies at ambient pressure conditions, in the pharmaceutical industry some operations are performed in supercritical conditions,

being the equations of state particularly useful for these studies. Therefore, the solubility of drug-like molecules in supercritical solvents using CPA EoS was estimated, namely for acetylsalicylic, adipic, ascorbic, nicotinic and stearic acids, acetamide, camphor, dibenzofuran, hexachlorobenzene, hydroquinone, ibuprofen showing again that this EoS is particularly useful for that kind of systems.

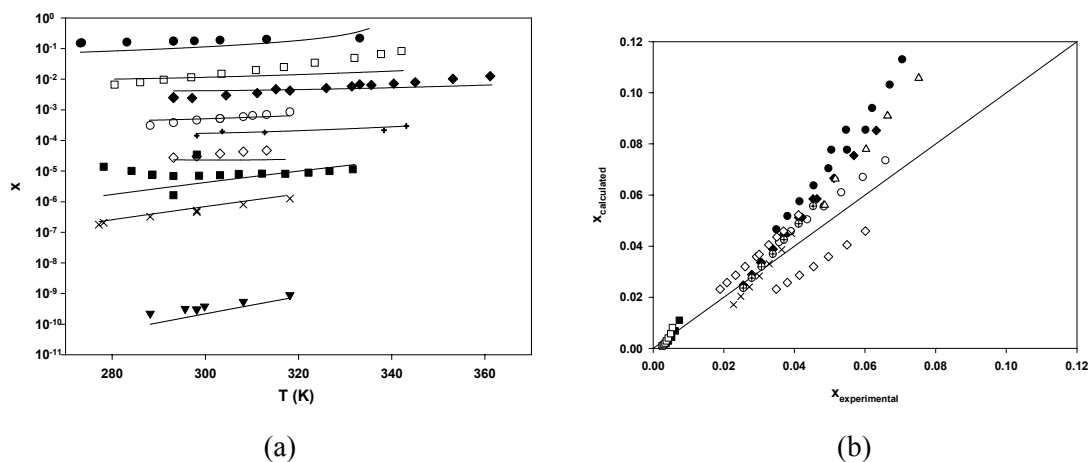


Figure 1. (a) Aqueous solubilities (\circ , acetylsalicylic; \blacklozenge , nicotinic; \blacksquare , terephthalic acids; \bullet , acetamide; \diamond , bisphenol A; $+$, camphor; \times , dibenzofuran; \square , hydroquinone; \blacktriangledown , hexachlorobenzene) and CPA results. (b) Summarized results for paracetamol in: \bullet , ethanol; \circ , methanol; \blacklozenge , 2-propanol; \diamond , acetone; \blacksquare , acetonitrile; \square , ethyl acetate; Δ , propylene glycol; \square , 1-propanol; \times , 1-butanol.

References

- [1] P. Kolář, J. W. Shen, A. Tsuboi, T. Ishikawa, *Fluid Phase Equilib.* 194 (2002) 771-782.
- [2] F. L. Mota, A. J. Queimada, S. P. Pinho, E. A. Macedo, *Fluid Phase Equilib.* 298 (2010) 75-82.
- [3] F. L. Mota, A. J. Queimada, S. P. Pinho, E. A. Macedo, *Fluid Phase Equilib.* (2011) accepted.