

20 SAFT 10

September 19-21, 2010, Barcelona, Spain

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# Book of Abstracts



**SPECIAL SYMPOSIUM**

**20 YEARS OF THE SAFT EQUATION:  
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## CPA EoS Modelling of Multifunctional Associating Fluids

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Molecules containing different associating groups such as amine, hydroxyl and carboxyl are important chemicals in the food, chemical and pharmaceutical industries. The thermodynamic properties as well as the phase equilibria involving such compounds are frequently modelled with group contribution models, such as UNIFAC. Still these models frequently miss some group interaction parameters, as well as have known limitations regarding aqueous systems or high pressures, for what associative equations of state have shown to perform better. In this contribution we will show how the Cubic-plus-Association equation of state (CPA EoS) can be employed [1,2] to represent the vapour-liquid, liquid-liquid, solid-liquid, liquid-gas and solid-gas equilibria of different multifunctional associating molecules such as phenolics, drugs, drug-like molecules and dicarboxylic acids in aqueous, organic and supercritical media.

[1] A. J. Queimada, F. L. Mota, S. P. Pinho, E. A. Macedo, *J Phys Chem B*, 113 (2009) 3469-3476

[2] F. L. Mota, A. J. Queimada, S. P. Pinho, E. A. Macedo, *Ind Eng Chem Res*, 47 (2008) 5182-5189