Surface Tension of Chain Molecules – A Combination of the Gradient Theory with the CPA EOS

M.B. Oliveira[1], I.M. Marrucho[1], J.A.P. Coutinho[1], G. M. Kontogeorgis[2], C. Miqueu[3] and A.J. Queimada[1,C, S]

[1]*CICECO, Chemistry Department, Aveiro University, Aveiro, Portugal*
antonioq@dq.ua.pt

[2]*IVC-SEP, Chemical Engineering Department, Technical University of Denmark, Lyngby, Denmark*

[3]*Laboratoire des Fluides Complexes, Université de Pau et des Pays de L'Adour, Pau, France*

A combination of the gradient theory of fluid interfaces with the Cubic-Plus-Association (CPA) equation of state was selected with the final aim of modeling vapor-liquid and liquid-liquid equilibria and interfacial tensions of systems containing associating and non-associating components such as alkanes, perfluoroalkanes, alcohols and water.

In this work, a broad pure component database was used to evaluate the equilibrium pressures, vapor and liquid densities as well as the surface tensions of the above-mentioned fluid families obtained with the selected model. The nature of the physical contribution in CPA (SRK or PR), will also be discussed.

Conclusions regarding the optimization and selection of the EOS parameters and the correlation of the pure component influence parameters will also be presented and discussed. Based on the results, considerations for the future modeling of multicomponent multiphase systems will be exposed.

Acknowledgements: This work was supported by Fundação para a Ciência e a Tecnologia through project POCI/EQU/58239/2004. A. J. Queimada acknowledges Fundação para a Ciência e a Tecnologia his post-doctoral (BPD/12871/2003) scholarship.