Poster SCF22

Modeling of the Solubility of Antilipemic Agents Using Different Peng-Robinson Equation of State - Mixing Rule Combinations

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Generally the main difficulty in calculating the solubilities of solid compounds in supercritical fluids is the choice of the most appropriate combination of an equation of state (EOS) and a mixing rule (MR), for the given conditions.

Consequently the present work is concerned with the modeling of the solubility of three antilipemic agents of clofibric acid, fenofibrate and gemfibrozil in supercritical carbon dioxide using Peng Robinson equation of state in combination with four different mixing rules, namely, that of van der Waals, Panagiotopoulos and Reid, Wong-Sandler and Kwak and Mansoori mixing rules.

A priori the required physicochemical and critical properties of the three antilipemic agents were predicted using well known methods based on the group contribution concepts.

The interaction parameters k_{ij} was obtained from experimental data reported in the literature and concerning the considered compounds, by the optimization of a well defined objective function using the Nelder-Mead version of the simplex technique.

Good agreement between the calculated and experimental data was obtained for few EOS-MR combinations only, confirming that the accuracy of the results depends upon the choice of the adopted combination.

Finally the model of the best EOS-MR combination can be used to perform computer experiments according to various specific applications like for instance the micronization process using supercritical fluid where thermodynamics and phase equilibrium are the key matters.