Interfacial Properties of Tetrahydrofuran (THF) and Their Mixtures with Some Compounds of Industrial Interest: Atomistic and Coarse Grained Molecular Simulation Models

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The accurate description of the phase equilibria and interfacial behavior of tetrahydrofuran (THF) and their mixtures with compounds of fundamental importance in processes related with natural gas hydrates recovery and CO2 storage, among many others, from a microscopic point of view is essential to understand how molecular details determined the macroscopic behavior of these mixtures. We combine the information obtained from the predictions obtained from the well-known SAFT-VR approach (Determination of the global phase behavior of THF + CH4, + CO2, and + H2O binary mixtures using the SAFT-VR approach), also presented in this conference, to determine the thermodynamic behavior of some mixtures containing THF. In particular, in this work we focus on the description of the interfacial behavior of these systems using two alternative approaches, atomistic molecular dynamics (MD) and coarse grained molecular dynamic (CG-MD) simulations. Agreement between the results obtained from different methods, including MD simulations and theoretical predictions from SAFT, and experimental data taken from the literature is analyzed in this contribution.