Vapour-liquid interfacial properties of tetrahydrofuran + carbon dioxide binary mixture from molecular dynamics simulation

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Tetrahydrofuran (THF) is a cyclic ether rutinely used as thermodynamic hydrate promoter that produces a pronounced shift on the hydrates coexistence curves when used as an additive. Different authors have used THF for applications as the reduction of the equilibrium pressure of carbon dioxide (CO_2) hydrates for environmental concerns related with greenhouse gas emission controal and effects on global climate change [1].

In this work we investigate the ability of different models of THF, when is mixed with CO_2, in predicting phase equilibria and interfacial properties before to use them for determining the equilibrium and structural properties of CO_2 hydrates with THF.

THF is modelled using two different molecular models based on the united-atom approach. The first model of THF considered is the original TraPPE-UA model propoused by Keasler *et al.* [2]. The second model of THF studied is an approximated, planar, and rigid TraPPE model [3], in which non-bonded LJ intermolecular parameters and partial charges located at the different chemical groups are identical to those of the original TraPPE model. CO_2 is modeled using the TraPPE model propused by Potoff and Siepmann [4].

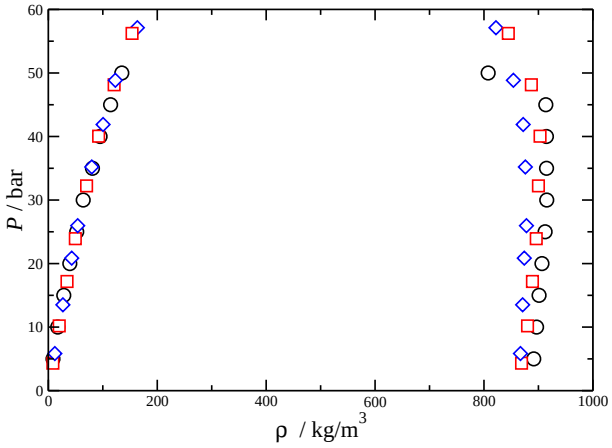

Figure 1: Vapour-liquid coexistence densities for the THF + CO_2 binary mixture at 298.15 K and several pressures. Open blue diamonds correspond to the coexistence densities obtained from MD-NVT simulations using the original TraPPE-UA model [5] and open red squares using the rigid TraPPE-UA model [5]. Open black circles are experimental data taken from the literature [6].

Molecular dynamics (MD) simulations have been performed in the NVT canonical ensemble using the MD package GROMACS [5]. Results have obtained obtained at different thermodynamic conditions and using the two molecular models for THF are presented in this work. In particular, we compare simulation results and experimental data taken for the literature, at two different temperatures and several pressures, for the vapour-liquid pressure-density and pressure-composition projections of the phase diagram, as well as interfacial tension as a function of pressures. Molecular simulation results are able to predict the experimental data taken from the literatue [6] for the equilibrium and interfacial behaviour of the mixture.

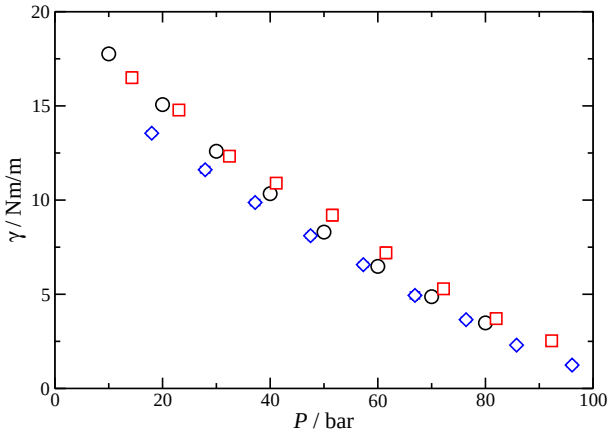

Figure 2: Surface tension for the THF + CO_2 binary mixtures at 353.15K as obtained from MD-NVT computer simulations. The meaning of the sysmbols is the same as in Figure 1.

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