Prediction of the Phase Behavior of the Tetrahydrofuran + Water Binary Mixture by Molecular Simulations

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Tetrahydrofuran is a cyclic ether widely used as solvent in many industrial processes. Among its diverse applications, it is used as thermodynamic clathrate hydrate promoter and that represents a particular motivation for the present study. Furthermore, an accurate description of phase equilibria of the tetrahydrofuran + water mixture is essential to understand the efficiency and efficacy of the latest application cited. The phase diagram of the binary mixture tetrahydrofuran + water exhibits a really interesting VI phase behavior according to the classification of van Konynenburg and Scott. This type of behavior is characterized by the presence of a Bancroft point, positive azeotropy, and the so-called closed-loop curves that represent regions of liquid-liquid immiscibility in the phase diagram. The system exhibits lower critical solution temperatures (LCSTs), which denote the lower limit of immiscibility together with upper critical solution temperatures (UCSTs). This behavior is explained in terms of competition between the incompatibility with the alkyl parts of the tetrahydrofuran ring chain and the hydrogen bonding between water and the ether group. Water is modelled using the well-known TIP4P/2005 water model and tetrahydrofuran is described using a rigid version of the original TraPPE model. Finally, predictions from computer simulations carried out in the NPzT ensemble are compared with experimental data taken from the literature.