Study of the Interfacial Properties of Water+1-Alkanols Binary Mixtures from Molecular Simulations

José Manuel Miguez [C, S] and Jesús Algaba Fernández
Centro de Investigación en Química Sostenible (CIQSO), Universidad de Huelva, Huelva, Spain
jose.miguez@dfa.uhu.es

Jose Matías Garrido
Departamento de Ingeniería Química, Universidad de Concepción, Concepción, Chile

Paula Gómez Álvarez and Felipe Blas
Centro de Investigación en Química Sostenible (CIQSO), Universidad de Huelva, Huelva, Spain

Interfacial properties of aqueous mixtures of 1-alkanols govern the efficiency and efficacy of several processes in chemical, petroleum, and environmental engineering sectors. Some particular cases in the chemical engineering field are those involved in interfacial mass transfer unit operations such as liquid extraction, extractive distillation, and interfacial chemical reactions. In these cases, the interfacial concentration and its surface activity (i.e., adsorption or enrichment of one component in the interface) have an important impact on the mass transfer of species through the interface region. In this work, we use molecular dynamics simulation to predict the interfacial properties of water + 1-alkanols that exhibit liquid-liquid immiscibility phase behavior. Water is modelled using the well-known TIP4P/2005 water model and 1-alkanols (from 1-butanol up to 1-octanol) are described using the original TraPPE models. In particular, we have considered the temperature dependence of the most important interfacial properties of these mixtures, including density profiles, phase coexistence diagrams, interfacial thickness, and interfacial tension as functions of temperature at atmospheric pressure. Predictions from computer simulations carried out in the PNzT ensemble are compared with experimental data taken from the literature. Finally, simulation results and experimental data are compared and discussed.