Structure of the Methanol/Water Vapor-Liquid Interface

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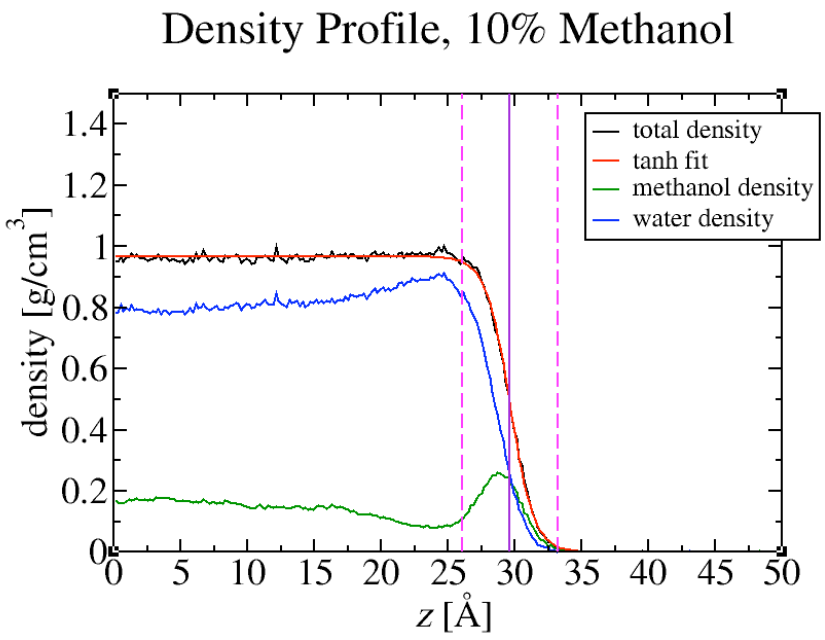
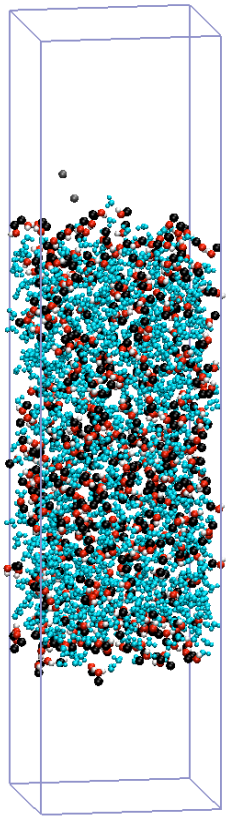
As part of a collaborative effort (together with researchers from the University of Minnesota, Lawrence Livermore and Pacific Northwest National Laboratories), we are contributing to a comprehensive particle-based study of the vapor-liquid interface of methanol/water mixtures. The overall study will compare different simulation techniques (Monte Carlo and molecular dynamics) and a range of models (from empirical molecular mechanics force fields to Kohn-Sham density functional theory) used to determine structural, thermodynamic, and dynamic properties of the liquid-vapor interface at three different compositions: 10% methanol, 20% methanol, and 30% methanol. The general aim is to investigate the composition dependence of the interfacial properties and to assess the transferability of current models to interfacial systems. Of particular interest is the performance of DFT models that, when combined with molecular simulation methods in a first principles approach, incorporate elements of quantum calculations (for example, the ability to make and break chemical bonds or to determine reactive frontier orbitals). Our specific contribution is to provide a benchmark interface using popular empirical force fields. We use the TIP4P model[1] for water and the TraPPE model[2] for methanol and perform configurational-bias Monte Carlo simulations in the Gibbs ensemble. Results for the empirical models are in good agreement with experimental data from recent surface-sensitive spectroscopic studies of similar interfacial systems.[3]





References:

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2. Chen, B.; Potoff, J. J.; Siepmann, J. I. *J. Phys. Chem. B*, **105**, 3093 (2001).
3. H. Chen, W. Gan, R. Lu, Y. Guo, and H-f. Wang *J. Phys. Chem. B*, **109**, 8064 (2005).