Molecular Simulation Studies on Alternative Fluoropropene Refrigerants

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Fluoropropenes such as HFO-1234yf or HFO-1234ze(E) are currently discussed as refrigerants for various applications, either as pure compounds or as components in low GWP refrigerant mixtures. However, studies on the performance of these new refrigerants in technical applications require information on various properties such as phase equilibria, transport and caloric properties over a wide range of state points. Thus, we developed a transferable molecular model (force field) for fluorinated propenes to enable reliable predictions for the thermophysical properties of this new class of alternative refrigerants and their mixtures by molecular simulation studies to complement experimental data. The all-atom force field model at that time comprises the compounds HFO-1234yf, HFO-1243zf, HFO-1216 as well as cis and trans isomers of HFO-1234ze and HFO-1225ye. The molecular model has been validated by Gibbs ensemble simulations on the vapor liquid equilibria of the compounds. Furthermore, we have tested the performance of the force field by molecular dynamics simulations on liquid phase properties such as densities or viscosities. We will also present studies on the local structures of the isomers HFO-1234ze and HFO-1234ze(E) to provide insight into their behavior on a molecular level. Our force field might be especially useful to provide predictions for the thermophysical properties of alternative refrigerant blends containing fluorinated propenes. Thus, we will also present first results on molecular simulation studies on mixtures of fluoropropenes with other compounds such as CO₂.