Molecular Simulation Studies on HFO Based Working Fluids

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Due to their low Global warming potential (GWP) different hydrofluoroolefins are currently discussed as working fluids for various applications, either as pure compounds or as components in blends. Though, studies on the performance of these new working fluids in technical applications require information on various properties such as phase equilibria, transport and caloric properties over a wide range of state points. On the 18th Symposium on Thermophysical properties in 2012, we have presented a transferable force field for fluorinated propenes [1, 2] that enables reliable predictions for the thermophysical properties of this new class of refrigerants and their mixtures by molecular simulation studies. This force field has also been applied to yield predictions on the VLE and liquid phase properties of mixtures of fluoropropenes such as HFO-1234yf, HFO-1234ze with other working fluids like R-32 or CO2, and for the refrigerant blend R-445A [3-5]. The force field model has now been extended to include chlorinated components such as HCFO-1233zd or fluorinated butenes such as HFO-1336mzz. Thus, we will present molecular simulation results for the thermophysical properties of different HFO compounds, and also of their mixtures with other working fluids. Our simulation studies comprise Gibbs Ensemble Monte Carlo simulations on the vapor-liquid equilibria, and molecular dynamics simulations on liquid phase properties such as densities or viscosities. We will thereby present simulation results for different compounds and blends that are currently proposed as working fluids for technical applications such as mobile air conditioning systems, heat pumps and ORC processes.

References

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