Molecular Modeling and Simulation Studies on HFO and HFCO Based Working Fluids

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Due to their low global warming potential (GWP), different hydrofluoroolefins have attracted attention as working fluids for various applications. Whereas the first HFO-based refrigerants mainly consisted on fluorinated propenes such as R-1234yf and R-1234ze(E), also fluorinated butenes and ethenes, as well as chlorinated compounds, so called hydrochlorofluoroolefines (HCFO), are currently proposed as alternative working fluids. As their commercialization is in its early stage, experimental data on the thermophysical properties of these newly introduced HFO or HCFO compounds are rare, and this hampers the exploration of their performance in potential technical applications. In 2009, we have started the development of a transferable force field for HFO and HCFO compounds to enable predictions of their properties by molecular simulations [1, 2]. Various simulations studies on pure HFO and HCFO compounds as well as on HFO based mixtures have already attested the performance and predictive ability of the force field model [1-5]. We will here provide an overview on the current state of the force field development and will present recent simulation results for the newly included compounds trifluoroethene HFO-1123 [6] and 1-chloro-2,3,3,3-tetrafluoropropene HCFO-1224yd(Z/E). The force field model also allows for predictive simulation studies on potential refrigerant blends, i.e. mixtures of HFO/HCFO compounds with conventional refrigerants such as R-134a, R-32 or CO2, or with other HFO/HCFO compounds. Thus, we will also provide an overview on the simulation studies on different HFO based mixtures that were already performed based on this molecular model. We will thereby present new simulation results for binary mixtures of HFO-1123 with R-32, R-1234yf, R-134a and R-1234ze(E), as well as for mixtures of R-1234yf with R-1234ze(E) and HFO-1336mzz(E).

References:

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