Molecular Modelling and Simulation Studies for Various HFO and HCFO Compounds and Their Mixtures

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Following the introduction of fluorinated propenes such as R-1234yf or R-1234ze(E) as low-GWP refrigerant, also hydrofluoroolefines (HFO) compounds based on fluorinated butenes as well as hydrochlorofluoroolefines (HCFO) are now discussed as alternative working fluids for different applications, such as high temperature heat pumps (HTHP), Organic Rankine Cycles or chillers. As for all newly proposed HFO and HCFO compounds, one faces the problem that experimental data for their thermophysical properties are rare, which hampers the evaluation of their performance in the potential technical application.

On the previous Symposiums on Thermophysical Properties, 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. We here present an approach for the extension of the molecular model to cover a wide range of HFO and HCFO compounds [3]. Based on this modelling approach we have performed purely predictive simulation studies on the vapour liquid equilibria of compounds such as 3,3,4,4,4-pentafluoro-1-butene (HFO-1345fz), 2,3,3,4,4,4-hexafluoro-1-butene (HFO-1336yf) and cis- and trans-1-chloro-2,3,3,3-tetrafluoropropene (HCFO-1224yd(Z/E)).

In addition to the results for the pure compounds, we will also present predictive simulation studies on binary mixtures of HFO and HCFO compounds, such as blends of trans-hexaflourobutene HFO-1336mzz(E) with its cis isomer, R-1234yf, or trans-1-chloro-3,3,3-trifluoropropene 1233zd(E).

References

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