New Parametrization Approach for Molecular Models, and Predictive Simulation Studies on Refrigerant Blends and Refrigerant-Lubricant Mixtures

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At previous Symposiums on Thermophysical Properties, we have presented a transferable force field for HFO and HCFO compounds [1-3] that enables reliable predictions for the thermophysical properties of this new class of working fluids and their mixtures by molecular simulation studies. However, the development of these force fields is a time-consuming and laborious endeavor. Thus, we have adopted and further developed the surrogate assisted optimization method based on Gaussian process (GP) regression introduced by Befort et al. [4] to parametrize a force field for the HCFO refrigerant *trans*-1,2-dichloroethene (R-1130(E)). Here, we present molecular simulation results for the VLE and viscosity of R-1130(E), and for the VLE of its mixture with R-1336mzz(Z).

Furthermore, we will present results from our ongoing work to provide predictions for new potential, but not yet well described refrigerant blends. Thus, we will present predictions from molecular simulations for the VLE properties of binary refrigerant mixtures such as R-1234yf-R1336mzz(E/Z), R-1234yf-R1234ze(Z), CO_2-R1234ze(Z), CO_2-R1336mzz(E/Z)), etc. The development of efficient and sustainable HVAC&R systems also requires a fundamental understanding of the interactions and resulting thermophysical properties of the refrigerant-lubricant pairing. Therefore, we will also provide predictions for the viscosities of refrigerant-lubricant mixtures, including diverse refrigerants (R-1234yf, HCFO-1233yd(E), R-32, CO_2) as well as different pentaerythritol ester lubricants with varying molecular structures (PEC, PEB).

References

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