Extensive Molecular Simulation Computation of Thermophysical Properties for Pure Component Refrigerant Molecules and Their Mixtures

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Seven refrigerant molecules namely, R14, R32, R50, R125, R134a, R143a, & R170, and one key refrigerant mixture, R-410a, were studied using molecular simulation (MS).

To sustainably phase out high global warming potential refrigerants, azeotropic or near-azeotropic refrigerant mixtures must be separated into their components. Ionic liquids (ILs) and deep eutectic solvents (DESs) are being proposed as entrainers for this difficult separation. MS is an important tool for the development of these refrigerant mixture separation technologies. However, before MS is applied to investigate complex systems of these refrigerant mixtures in ILs or DESs, it is important to rigorously study the thermophysical properties of the pure components and mixtures of these refrigerant molecules using MS. This will help to validate force fields (FFs) for these refrigerant molecules, develop/validate best practices for computing the plethora of thermophysical properties required for developing these separation technologies and provide a basis for a fundamental understanding of the more complex IL/HFC or DES/HFC systems.

Thermal conductivity, viscosity, self-diffusivity, isobaric and isochoric heat capacities, isothermal compressibility, thermal expansivity, thermal pressure coefficient, Joule-Thomson coefficient, sonic speed, and surface tension were calculated using FFs previously developed by our group for each of the systems studied across multiple state points. MS results were compared with the National Institute of Standards and Technology (NIST) data. Results show generally excellent agreement with NIST values for all the systems and properties studied. The average of the mean absolute percentage deviations was generally within 10 % for most of the systems studied. The FFs for R14, R50, and R170 however showed limited qualitative predictive accuracy of the thermal conductivity. This calls for further investigation.

This work provides a comprehensive set of molecular simulation results on the thermodynamic, transport, and interfacial properties across multiple state points for seven refrigerant molecules and one critical refrigerant mixture.