Modeling Thermodynamic and Transport Properties of Hydrogen-Containing Mixtures

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Hydrogen, as a clean and efficient energy carrier, plays an important role in the transition to low-emission energy utilization. Accurate modeling of thermodynamic and transport properties of hydrogen-containing mixtures is essential for hydrogen energy applications, but is challenging because of the quantum effects and very low critical temperature yielding strongly asymmetric mixtures. In this work, the thermodynamic and transport properties of hydrogen-containing mixtures are modelled using the volume-translated PR equation of state (VTPR EoS) [1, 2], quantum-corrected PR (PRQ) EoS [3], and PC-SAFT EoS [4]. Then, these models are combined with the residual entropy scaling (RES) [5] approach for modeling transport properties. A critical review of experimental data is conducted for binary mixtures containing hydrogen, including vapor-liquid equilibria (VLE), density, caloric properties, viscosity, and thermal conductivity. The EoS and RES models are evaluated using the curated database. The PC-SAFT model is re-parameterized so that the critical pressure of pure fluids and VLE incorporating a supercritical fluid (hydrogen) can be accurately represented. Advantages of the PC-SAFT compared to the cubic EoSs are discussed.

References

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