An Equation of State Based upon a Rational Form for the Residual Helmholtz Free Energy

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Chemical process modeling and design requires accurate equations to predict energies, entropies and densities. Cubic equations of state have a simple form that can describe thermophysical properties making assumptions that increase error in the prediction. In other hand, recent multi parametric equations can predict thermodynamic properties with high accuracy by increasing the calculation complexity. This work presents a new equation of state (EoS) having a rational form that can describe properties with accuracy comparable to the best multi-parametric equations with less mathematical complexity. This EoS presents the Helmholtz residual energy as a ratio of two polynomial functions in density (no exponential terms in density are included), which can describe the behavior of pure components. The EoS needs 32 parameters to describe a pure fluid. The EoS can be transformed to describe other thermophysical properties as pressure, compressibility factor, heat capacity and speed of sound.

As one example, this work describes nitrogen data from 66 to 520 K at pressures up to 30 MPa. The equation can predict compressibility factors within 0.02% for temperatures between 130 K and 520 K. For temperatures below the critical point the uncertainty is around 0.05%, and within the critical region the uncertainty is higher. The model estimates saturated densities within 0.05% for temperatures below 125 K. This EoS also describes reported speed of sound and heat capacity measurements within 1% everywhere except the near critical region.