

Universal Cubic Equation of State for Modeling Thermodynamic and Transport Properties of Fluids and Fluid Mixtures

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The scientific goal is to achieve the modelling of the thermodynamic (vapor pressure, saturated liquid densities, single-phase liquid densities, compressibility factor, HPHT phase equilibria, interfacial tension, isobaric compressibility, volume expansivity, enthalpy, entropy, internal energy, Gibbs free energy, isobaric and isochoric heat capacities, Joule-Thomson coefficient, speed of sound) and transport (dynamic viscosity, kinematic viscosity, thermal conductivity, thermal diffusivity, molecular diffusivity, dielectric constant, Prandtl number and Eucken number) properties within a single functional framework of applying the same set of parameters used in thermodynamic equation of state in the transport equation of state model. Such a goal has been achieved by the reformed Van der Waals 1873 cubic equation of state, which hereafter has been named the Lawal-Lake-Silberberg (LLS) cubic equation of state. The LLS equation is designed with four physically meaningful parameters that reflect molecular attraction, size, structure and shape for the individual pure substances and it is applicable for predicting thermodynamic and transport properties over the entire PVT states, including fluid vapor-liquid critical point. The thermodynamic equation of state is unified with the caloric and transport equations of state through the judiciously designed Van der Waals Gas-Constant (R_{vdw}) for ideal-gas behavior. While the LLS equation is built with two continuously differentiable attractive and repulsive temperature functions $a(T)$ and $b(T)$, we are still lacking the generality for the three binary interaction parameters that relate the pure component parameters and composition to the mixture combining rules that are specified for the attractive parameter a_m and two other parameters that relate the critical compressibility factor predicted by the LLS equation to the composition of mixture thereby guaranteeing stable convergence of gas-liquid properties at far away from, neat to and at the critical point of mixture of fixed overall composition. The versatility of the LLS cubic equation is illustrated with the prediction of accurate volumetric and coexistence gas-liquid densities of asymmetric pure components and the prediction of accurate phase equilibria, saturated liquid densities and critical properties of binary systems.