# Symbolic Regression Used to Develop a New Cubic Equation of State for Improved Liquid Density Calculations

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For over a century, cubic equations of state (EoS) have been used to calculate phase behavior, density, and residual properties (e.g., residual entropy) of pure fluids and mixtures. They have a reasonable balance of simplicity, accuracy, and generality and thus are commonly used in industry. Despite a century's development with hundreds of resulting cubic EoS, the accuracy of liquid-phase density calculation using cubic EoS is still unsatisfactory. In this work, based on the form of the Patel-Teja (PT) EoS:

$$p = \frac{RT}{v-b} - \frac{a\alpha(T)}{v(v+b)+c(v-b)}$$

we present a new cubic EoS aiming at an improved liquid density calculation. Almost all pure fluids in the NIST REFPROP database version 10.0 are studied, and calculations of REFPROP 10.0 are used as reference values. The PT EoS is a generalized three-parameter cubic EoS, which can be reduced to popular EoS like Soave-Redlich-Kwong (SRK) and Peng-Robinson (PR). In the original PT EoS, parameters a, b, and c are linked to an empirical critical compressibility factor $\xi_C$, and all four of these parameters are constants for a pure fluid. In our new equation, $\xi_C$, *a*, *b*, and *c* are functions of temperature in the form of an equation developed with symbolic regression and the internal parameters are optimized with nonlinear regression. The form of $\alpha(T)$ is the popular Soave form, as it is subject to many constraints and does not obviously affect the liquid-phase density calculation. Temperature, pressure, and density data at saturated and homogenous states are used in the optimization. As a result, the average of the absolute value of relative deviations (AARD) of liquid-phase density calculated with the new EoS from reference values is reduced to approximately 1%, compared to 2% when using the Patel-Teja-Valderrama (PTV) EoS and 4% with the PR EoS. Meanwhile, predicting other properties (phase behavior and residual properties) is generally similar to or slightly better than the PTV, SRK, and PR EoS.