Development of a Five-Parameter Cubic Equation of State

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A new five-parameter cubic EOS is developed from PVT and saturation data for over 150 compounds, including light gases, hydrocarbons, halogenated refrigerants, alcohols, quantum and other fluids. The EOS parameters comply with geometrical criteria (Schmidt and Wenzel, 1980; Olivera-Fuentes, 1989; Santos and Olivera-Fuentes, 1995a) to ensure that the covolume parameter is consistently the largest pole on the PV plane. The classical stability conditions are imposed at the critical point, honoring the experimental critical volume. Subcritical parameters are determined by a combination of Abbott's (1979) algebraic procedure and a gradient search technique (Santos and Olivera-Fuentes, 1995b), thus guaranteeing exact reproduction of experimental saturation pressures and volumes, and best overall fit of the subcritical isotherms. The gradient technique alone is used at supercritical conditions.

Generalized correlations are developed for the five EOS parameters in terms of reduced temperature, acentric factor and dipole moment. A sequential procedure is used, in which each of the parameters is fitted in turn, the remaining parameters being then recomputed for all compounds to minimize the loss of accuracy introduced in the regression procedure.

Comparisons with traditional cubic EOS (Soave-Redlich-Kwong, Peng-Robinson and Patel-Teja) and with the few other five-parameter cubic EOS available in the literature (Kumar-Starling, Adachi and modified Kumar-Starling) show that the new EOS gives better predictions of saturated liquid properties, and provides better representation of the critical isotherm and near-critical region. Predicted supercritical volumes and enthalpies are also in good agreement with experimental values, even for polar and quantum fluids. However, because of the different fitting techniques used in the subcritical and supercritical regions, a discontinuity is introduced in the predicted enthalpies at the critical temperature.