

A Generalized Cubic Equation of State for Non-Polar and Polar Substances

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A generalized cubic equation of state (EoS) to describe vapor pressure and liquid densities of polar and non-polar substances is developed. The EoS is based on the Peng-Robinson pressure-volume-temperature relationship, the alpha function of Heyen and it is a two-parameter EoS in terms of the critical temperature, the critical pressure, the acentric factor and the polar factor of Halm-Stiel. The EoS was developed using two vapor pressure data for 67 highly polar compounds and 23 n-alkanes. To validate the EoS, vapor pressure was calculated for 181 polar and 82 non-polar compounds. The average absolute relative deviation obtained is 1.51%. In total, 8463 vapor pressure were calculated for polar substances and 2300 for gases and hydrocarbons. The EoS was compared with a modified Patel-Teja (PTH) EoS that requires substance-dependent parameters, the Peng-Robinson (PR) EoS and a generalized version of the Peng-Robinson-Stryjek-Vera (PRSV) EoS. Results show that the new EoS is superior to the generalized EoS and it is similar to the PTH EoS that only correlates the experimental data. The deviations are 6.18%, 6.66% and 1.27% for the PR, the PRSV and the PTH EoSs. Additionally, to improve liquid densities estimations, the EoS was translated in volume using one saturated liquid volume. The translation-parameter was generalized for gases and hydrocarbons and it was estimated for polar compounds. Saturated liquid densities calculations were performed for 285 substances and deviations are below 2.8%. Similar values correspond to the PTH EoS. Finally, single-phase density calculations including pressures above 100 MPa were performed for 13 alkanes. Results are better with the proposed model, especially for heavy hydrocarbons. For example, the deviation for n-tetracosane is 6.2% using the proposed EoS while for the PR and the PTH are 44.8% and 13% respectively. Similar results are obtained for other compounds like n-eicosane and n-octacosane.