

Improvement of the Two Parameter Cubic Equation of State to represent vapor pressure of pure compound

L.A. Galicia-Luna C, S

Laboratorio de Termodinámica, Instituto Politécnico Nacional, México D.F., Mexico
lagalicia@netscape.net

Equations of State are important to represent global phase diagram of mixtures from the theoretical and experimental point of view and especially in the design and modeling of supercritical processes in the oil, Pharmaceuticals and chemical industry. Precise vapor pressures representation of polar and nonpolar pure compounds is required to improve the robustness of equation of state to predict phase equilibria of mixtures. In this paper the Soave [1] and Peng-Robinson [2] equations of states has been modified to improve its accuracy. It was modified their temperature dependence of the attraction term for both equations of state to reproduce accurately vapor pressure (less than 1 %) of 341 pure compounds containing alkanes, alcohols, refrigerant, and sulfur compounds.

[1] G. Soave, Chem. Eng. Sci., 27, 1197 (1972).

[2] D. Y. Peng, and D. B. Robinson, Ind. Eng. Chem. Fundam. 15, 59(1976).