Thermodynamic Properties Calculations by Modified MMM (M4) Equation of State

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Abstract:

The modified MMM equation of state (M4 EOS) has been proposed in a previous work. In this work the application of this EOS is extended by presenting the enthalpy of vaporization for 54 pure compounds and VLE calculations for 50 binary mixtures. The results are compared by those obtained by Peng-Robinson and Soave Redlich-Kwong equations of state. The Average Absolute Deviation (AAD%) from the experimental results for modified MMM EOS was lower than the other two EOSs.

Introduction:

Mohsen-Nia et al., developed a new cubic equation of state (M4 EOS)[1] as:

$$Z = \frac{V + kb}{(V - b)} - \frac{a}{RT^{3/2} V(V + Nkb)} \qquad (1)$$

$$k = 1.3191$$

There are two constrains for selection of a value for parameter N:

1. The maximum packing fraction for different fluids must be less than $y = b/4V = 0.35$, [2].
2. The critical compressibility factor (Z_c) must match the average critical compressibility factor of real fluids (about 0.3).

With regard to the above considerations, we choose N=2; therefore, the proposed equation of state (M4 EOS) is in the following form:

$$Z = \frac{V + kb}{(V - b)} - \frac{a}{RT^{3/2} V(V + 2kb)} \qquad (2)$$

By imposing the critical point constrains, the following expressions have been derived:

$$a_C = 0.47312\, R^2 T_C^{2.5} / P_c \qquad (3)$$

$$b_c = 0.04616\, RT_c / P_c \qquad (4)$$

$$Z_C = 0.308 \qquad (5)$$

The accurate prediction of vapor pressures and liquid densities of fluids, by two parameter cubic equations of state can be enhanced by choosing the appropriate temperature and