Development of a Novel Equation of State (EoS) Model

Ilya Polishuk, Department of Chemical Engineering and Biotechnology, Ariel University Center, Ariel, Israel

So far the engineering models such as the cubic EoSs has been mostly focused on the accurate description of certain pure compounds properties, such as the liquid molar volumes and vapor pressures. However, this approach cannot satisfy anymore the requirements of the industrial process design and the need of considering other thermodynamic properties is evident. Presently we consider several properties which are inter-related though thermodynamic relationships, namely the 2nd and the 3rd virial coefficients, the Joule-Thomson Inversion curves, the isochoric and isobaric heat capacities.

All known van der Waals-type models erroneously predict the increase of the third virial coefficient at low temperatures. After some algebra the following generalized expression for the virial coefficients can be derived:

$$c_i = \frac{\lim_{\rho \to 0} \left(\frac{\partial Z^{i-1}}{\partial^{i-1} \rho} \right)}{(i-1)!}$$

where c_i is the i-th virial coefficient. This expression suggests the following form for the EOS:

$$P = \frac{RT}{V} f(\eta) - \frac{a(T)\left(V + d(T)\right)}{(V+c)^3}$$

Where η is the packing fraction and a, c and d are the EoS's parameters. An appropriate evaluation of these parameters allows correct orediction of the 3rd virial coefficient and considerable improvement in description of other thermodynamic properties.