

# Development of a Novel Equation of State (EoS) Model

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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 through thermodynamic relationships, namely the 2<sup>nd</sup> and the 3<sup>rd</sup> 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:

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

where  $c_i$  is the  $i$ -th virial coefficient.

This expression suggests  
the following form for the EOS:

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

Where  $\eta$  is the packing fraction and  $a$ ,  $c$  and  $d$  are the EoS's parameters. An appropriate evaluation of these parameters allows correct prediction of the 3<sup>rd</sup> virial coefficient and considerable improvement in description of other thermodynamic properties.

