

148m Global Parameter Optimization for Equations of State

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Most equation of state parameters are determined by performing a least squares fit of pure component liquid density and vapor pressure data. To more accurately represent mixtures, a binary interaction parameter is often determined based on mixture vapor-liquid equilibrium data. In order to more accurately predict the phase behavior of a range of fluids, the pure component parameters need to be representative of the behavior of that fluid in a variety of mixtures. One approach to achieve this is to simultaneously use mixture and pure component data in the fitting process. This can be accomplished by employing parallel computing and global optimization routines. Preliminary results of this approach in determining parameters for the polar PC-SAFT equation of state will be presented.