ABSTRACT

An Investigation of Binary Interaction Parameters
For Use with Cubic Equations of state

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Cubic equations of state (EOS) often fail to adequately describe phase behaviour in the critical region. This failure may be, in part, due to an inadequate selection of the value of the binary interaction parameter k_{ij}. In this research semi-empirical correlations for use with the Peng-Robinson (PR) EOS, which account for the pressure and temperature dependence of the binary interaction parameter from low pressures all the way to the critical region were developed.

Two separate binary interaction parameters, one for the liquid phase (k_{ij}^{l}) and the other for the vapour phase (k_{ij}^{v}) were postulated. Both these parameters were assumed to be related by the simple functionality $k_{ij}^{l} = \alpha.k_{ij}^{v}$ with the value α being dependent on the mixtures' temperature and reduced pressure and possessing a value of one (1) at the critical point.

k_{ij}^{l} and α correlated well with reduced system pressure and temperature. These correlations are however empirical being derived from experimental data and accordingly are subject to the limitations of such correlations.

Despite these limitations, significant improvements in phase compositions both away from and in the critical region, were obtained for binary hydrocarbon-hydrocarbon mixtures, hydrocarbon-CO_2 and hydrocarbon-N_2 system when the proposed correlations were utilised.

Keywords: Brent Anthony Gormandy, Binary Interaction Parameter(s), Isothermal Flash, Critical Region, Equation of State.