138e Generalized Cubic-Plus-Association Equation of State

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From the practical point of view it is desirable to employ a general model determined from pure compound properties, which at the same time account for the association effects. A convenient approach to satisfy this requirement is to employ the concept of association in conjunction with an equation of state. An equation of state, which combines the physical term of the classical SRK equation of state (Soave, 1972) with the association term based on the perturbation theory of Wertheim (1984, 1986), was developed as the Cubic Plus Association (CPA) equation of state (Kontogeorgis et al., 1996). Since only limited molecules were provided for these specific molecule-dependent parameters, the application is expected to the other substances than those whose parameters are available. The corresponding-states principle provides a useful method to correlate the properties and also to represent the physical behaviors; as a result, in this work we apply the extended corresponding-states method into the CPA so that it is to obtain a general CPA equation of state after its combination with the corresponding-states principle. The cubic-plus-association theory (CPA) is developed into a general equation of state in which the three pure-component parameters required for nonpolar molecules and five pure-component parameters for associating molecules are correlated by the extended corresponding-states theory. A comparison of the experimental vapor-pressure and liquid-density data for some representative molecules shows that the thermodynamic properties of any molecule may be predicted from this generalized CPA equation of state.