Thermodynamic Modeling of Phase Equilibrium and Thermophysical Properties of Multicomponent Sub- And Supercritical Fluids

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A large family of thermodynamic models suggested for calculations of phase and chemical equilibria and thermophysical properties of fluids use cubic equations of state. These equations make a nice instrument for the calculations of thermodynamic properties and phase equilibria of multicomponent non-ideal mixtures. The Redlich-Kwong-Soave (RKS) equation of state with modified binary interaction coefficients is used, in this work, as a uniform thermodynamic model for these purposes.

Thermodynamic models are also used for calculations of the critical points, phase boundaries, and metastable states of multi-component mixtures. The phase diagrams obtained include the boundary of mechanical stability, the spinodal that characterizes the boundary of diffusive stability, and the binodal. Note that the spinodal passes through the critical point of the mixture. The phase boundaries (interfaces) were calculated using the homotopy method.

Thermodynamic models were also used, in order to calculate the enthalpies and heat capacities of multicomponent mixtures, the heat effects of chemical transformations, and the values of adiabatic heating of the mixtures in critical regions. The data obtained show a possibility of describing anomalous behavior of the indicated properties of the mixtures in the supercritical region. Examples of calculating the phase diagrams, partial molar properties, and heat capacities of individual components and entire mixture are given.

The results obtained allow for the suggestion that the particular behavior of a fluid's thermophysical properties in the critical region most likely affects the progress of chemical processes in the reactors.