

Modeling and Calculation of Thermodynamic Properties and Phase Equilibria of Oil and Gas Condensate Fractions Based on Two Generalized Multiparameter Equations of State

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Based on two previously obtained generalized equations of state, which describe the properties of hydrocarbon chain and cyclic structures, a method for the predictive calculation of thermodynamic properties and phase equilibria of complex hydrocarbon mixtures (oil and gas condensate fractions) has been developed. The method is applicable over a temperature range from freezing to 700 K at pressures up to 100 MPa, including the liquid and gas phases, and the supercritical region. The calculation of thermodynamic properties is made within the framework of the extended three-parameter corresponding states principle. The acentric factor was chosen as the determining criterion of similarity. The complex hydrocarbon mixture is treated as an individual substance, known from physical chemistry as a single-fluid model. In this model, the mixture is a hypothetical individual hydrocarbon with an effective molar mass M and pseudocritical properties T_{pc} , p_{pc} , and ρ_{pc} . This hydrocarbon is characterized by the content of paraffin and cyclic structures in an effective molecule. The paper outlines the method and the results of testing on more than 300 oil and gas condensate fractions. In addition, the results obtained from cubic equations and a generalized equation of Kessler and Lee is presented. For the calculation of phase equilibria, a method for modeling the composition of complex hydrocarbon mixtures using pseudocomponents (subfractions) has been developed based on the distillation curve and a minimum set of physical and chemical properties of mixtures consisting of average boiling temperature, relative density, and molar mass. Rules for the transition from the single-fluid model of the substance used to calculate thermodynamic properties to the linear model of the mixture, from which phase equilibria can be calculated, have been developed. The phase equilibria results (dew points and bubble points) for the hydrocarbon mixtures from the proposed methods and cubic equations are presented. The accuracy of the predictive calculation of phase equilibria is approximately the same for both the multiparameter and the cubic equations of state. However, the accuracy of other thermodynamic properties, such as density, from the multiparameter equation is substantially better.