Generalized Equation of State for the Cyclic Hydrocarbons over a Temperature Range from the Triple Point to 700 K with Pressures Up to 100 MPa

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Hydrocarbons with cyclic structures (naphthenic and aromatic) make up a significant share of the hydrocarbon composition of oil and gas condensates, and are important for chemical technology. For the lighter aromatic and naphthenic hydrocarbons, a fundamental equation of state, which allows the calculation of all thermodynamic properties, has been developed. Reliable experimental data are not readily available for more complex hydrocarbons, and it is not always possible to develop dedicated equations of state for each compound. Thus, the development of a generalized equation is a good alternative. A critical analysis and selection of the most reliable experimental data for thermodynamic properties of naphthenic and aromatic hydrocarbons was made by the authors. The lack of experimental data in some regions of the state parameters was filled by calculated data. The inclusion of calculated data in the fitting procedure increased the stability of the equation and improved the extrapolation behavior. These data were included in the fitting procedure with small weights. The generalization is made possible through a framework of the extended three-parameter corresponding states principle. This equation is explicit in the reduced Helmholtz free energy, with the reduced density, reduced temperature, and acentric factor as independent variables. The acentric factor was chosen as the determining criterion of similarity. To describe the residual part of the reduced Helmholtz energy, an optimized functional form developed by Sun and Ely was used. This form was successfully used in previous work by the authors to develop a generalized equation of state for n-alkanes. Optimization of the coefficients and temperature exponents of the proposed equation took place simultaneously in a nonlinear form. The proposed equation has enough precision to calculate thermodynamic properties and phase behavior of the investigated hydrocarbons over a range of the acentric factor ω = 0.2 – 1.1 and over a temperature range from the triple point to 700 K with pressures up to 100 MPa.