Fundamental Equation of State for *n*-Octane

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The accurate knowledge of thermodynamic properties is a fundamental aspect of the development and optimization of energy and process technologies. However, experimental measurements of these properties are time-consuming and expensive. Furthermore, they are not available for every state point, which is needed in process simulations. Therefore, equations of state are used to provide the required thermodynamic properties. In this work, an equation of state for *n*-octane is presented. *N*-octane is the eighth n-alkane of the homologous series and belongs to the aliphatic and saturated hydrocarbons. It is mainly obtained by fractional distillation during the processing of petroleum and is used in solvents and cleaning agents. Furthermore, *n*-octane and its branched liquid isomers are elementary components of fuels and lubricating oils. In particular, it is also a trace element of typical natural gas mixtures. For future investigations of natural gas mixtures, the accurate description of each pure component is essential. The current equation of state for *n*-octane of Span and Wagner[1] was developed by an approach simultaneously addressing more than 15 different fluids. It is based on a generalized functional form for nonpolar fluids. For the adjustment of the fluid-specific coefficients for *n*-octane, the authors applied 22 datasets including mostly homogeneous density and vapor-liquid equilibrium data. Only few reliable data for caloric properties were considered and data at pressures above 100 MPa were not considered for the development of these “technical equations of state” on principle. Based on modern fitting techniques, a new equation of state was optimized to represent the available data within their experimental uncertainties. More than 7300 data points of different thermodynamic properties from 358 publications were applied to the fitting procedure. The resulting equation of state is valid from the triple point temperature T_{tr} = 216.37 K to T_{max} = 730 K with a maximum pressure of p_{max} = 980 MPa. Correct physical extrapolation behavior, which is important for the application to mixture models, was ensured by the analysis of numerous thermodynamic properties.

References

[1]. Span R., Wagner W., *Int. J. Therm. Physics*, 2003, 24: 41-109