New Methods for Fitting Equations of State with Application to cis-Decalin

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In response to technological developments related to carbon neutrality, new materials for various working fluids, refrigerants, and organic hydrogen carriers have been proposed over the past few years. It is necessary to develop various energy conversion processes along with absorption and distillation processes for hydrogen and other substances, and to improve their thermal efficiency. There is thus an urgent need to develop precise equations of state for these new fluids that can accurately reproduce limited measured information but can correctly reproduce vapor-liquid equilibrium and supercritical region properties far beyond measured states, including the behavior in the metastable region. In this study, we report the application of the latest fitting techniques for the Helmholtz energy type equation of state to *cis*-decalin, one of the candidate organic hydrogen carriers.

Specifically, we present the measured information used as input data for the present fitting (including the measured *PVT* properties in the liquid phase region obtained in this study), as well as guidelines for adjusting the parameters of the equation of state and critical constants, with the use of the new equation of state for *cis*-decalin that we have developed. Methods of modifying the equation of state parameters through visual observation of multiple properties to assure thermodynamic consistency over the entire fluid-phase region with the latest constraints will also be presented.