Quantification of Uncertainties in Experimental Data for Thermodynamic and Transport Properties

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Accurate physical property data is crucial in process and pipeline design, and it can be challenging to obtain reliable thermodynamic and transport properties for various conditions of temperatures, pressures, and compositions encountered during the simulation process. Although resources exist to aid in the evaluation of experimental data at NIST, AIChE DIPPR consortium, and many contract measurement laboratories, the corresponding states principle holds more promise in this area and provides another technique to complement the computer simulation methods. One of the deductions from the van der Waals theory of cubic equations of state, the Law of Corresponding States (LCS), is used to validate the accuracy in experimental data designed to predict physical properties, especially for substances that have never been studied experimentally. The LCS method is very suited for many industrially required organic fluids and mixtures without a limitation of the size, shape, or polarity of the fluids. As a matter of fact, more substances obey the LCS than many methods designed to predict the physical properties of the fluids.

A generalized four-parameter equation of state (EoS) is used to establish reduced equations of state for pure substances and mixtures, and several plots of the compressibility factor against the reduced temperatures and pressures are prepared, in order to evaluate variations in the measured data from various laboratories. In lieu of accurate critical volume data, an algorithm is developed via critical constraints imposed on the EoS, and closed-form equations are developed for predicting the critical volumes of substances and mixtures. These predicted critical volumes (derived by matching the measured critical temperature and critical pressure) reveal the range of errors (10 to 65 %) in the experimentally measured binary and ternary critical volumes. This EoS is an accurate and easy-to-use tool for the prediction of physical properties of fluids, and can be used to obtain insight for systems whose behavior is dominated by non-bonded interactions between chemical species. The EoS is also used to establish respective reduced viscosity and reduced thermal conductivity equations of state. These reduced transport property equations of state are utilized to evaluate the errors in the experimentally measured viscosity and thermal conductivity data. The range of errors (20 to 75 %) within measured transport property data from several laboratories is much higher than those observed in thermodynamic property measurements. In contrast to the average deviations, which do not show a complete picture of experimental scatter, the plots of the reduced thermodynamic and transport properties versus reduced temperatures and pressures reveal uncertainties and internal consistency within data from various laboratories around the world.