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Physical and thermodynamic properties of pure compounds and their mixtures play an important role in design, simulation and optimisation of chemical processes. The accuracy of process design and simulation largely depends on the accuracy of the underlying physical and thermodynamic data and property prediction models. While use of experimentally measured values for the needed properties is desirable in process design, the experimental data for the compounds of interest may not be available in many cases. Therefore, development of efficient and reliable property prediction methods and tools that can also provide estimates of uncertainties in predictions of properties and their effects on process design becomes necessary. For instance, the accuracy of design of distillation column to achieve a given product purity is dependent on many pure compound properties such as critical pressure, critical temperature, acentric factor etc. In such cases, accurate property values along with uncertainty estimates are needed to perform sensitivity analysis and quantify the effects of these uncertainties on the process design.

The objective of this work is to develop a systematic methodology to provide more reliable predictions with a new and improved set of model parameters for GC (group contribution) based and CI (atom connectivity index) based models and to quantify the uncertainties in the estimated property values from a process design point-of-view. This includes: (i) parameter estimation using available GC based and CI based property prediction models and large training sets to determine improved group and atom contributions; (ii) uncertainty analysis of property prediction models to establish statistical information such as covariance, standard error and confidence intervals; and (iii) use the results of uncertainty analysis to predict the uncertainties in process design. For parameter estimation, large data-sets of experimentally measured property values for a wide range of pure compounds are taken from the CAPEC database. Classical frequentist approach i.e., least square method is adopted for the estimation of model prediction uncertainties. The developed methodology provides property values along with uncertainties for the following 20 properties: normal boiling point, critical temperature, critical pressure, critical volume, normal melting point, standard Gibbs energy, standard enthalpy of formation, standard enthalpy of fusion, standard enthalpy of vaporization at 298 K and at the normal boiling point, entropy of vaporization at the normal boiling point, surface tension at 298 K, viscosity at 300 K, flash point, auto ignition temperature, Hansen solubility parameters, Hildebrand solubility parameter, octanol/water partition coefficient, aqueous solubility, acentric factor, and liquid molar volume at 298 K. The performance of property models for these properties with the revised set of model parameters is highlighted through a set of compounds not considered in the regression step. The comparison of model prediction uncertainties with reported range of measurement uncertainties is presented for the properties with related available data. The application of the developed methodology to quantify the effect of these uncertainties on the design of different unit operations (distillation column, liquid-liquid extraction, heat exchanger, crystallizer, equilibrium reactor etc.) is presented. The results show that depending on the chemical systems involved and the operating conditions being considered, some of the input uncertainties can result in significant uncertainties in design. The most sensitive properties for each unit operation are also identified. This analysis can be used to reduce the uncertainties in property estimates for the properties of critical importance (by performing additional experiments to get better experimental data and better model parameter values). Thus, the developed methodology can be used to quantify the sensitivity of process design to uncertainties in property estimates; obtain rationally the risk/safety factors in process design; and identify additional experimentation needs in order to reduce most critical uncertainties.

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