Effect of Uncertainties in Physical Property Estimates on Process Design - Sensitivity Analysis

Amol Hukkerikar [S], Mark Jones, Gürkan Sin and Rafiqul Gani [C]
Technical University of Denmark, Computer Aided Process-Product Engineering Center (CAPEC), Department of Chemical and Biochemical Engineering, Lyngby, Denmark
rag@kt.dtu.dk

Chemical process design calculations require accurate and reliable physical and thermodynamic property data and property models of pure components and their mixtures in order to obtain reliable design parameters which help to achieve desired specifications. The uncertainties in the property values can arise from the experiments itself or from the property models employed. It is important to consider the effect of these uncertainties on the process design in order to assess the quality and reliability of the final design. The main objective of this work is to develop a systematic methodology for performing sensitivity of process design subject to uncertainties in the property estimates. To this end, first uncertainty analysis of the property models of pure components and their mixtures was performed in order to obtain the uncertainties in the estimated property values. As a next step, sensitivity analysis was performed to evaluate the effect of these uncertainties on the process design. The developed methodology was applied to evaluate the effect of uncertainties in the property estimates on design of different unit operations such as extractive distillation, short path evaporator, equilibrium reactor, liquid-liquid extraction, crystallizer etc. The sensitivity of design parameters to uncertainties in the property estimates was performed using one-factor-at-a-time approach. The results showed that depending on the pure components and their mixtures involved, the driving forces they represented, the operating conditions, and the choice of the property prediction models, the input uncertainties resulted in significant uncertainties in the final design. The developed methodology was able to: (i) assess the quality of final design; (ii) identify pure component and mixture properties of critical importance from a process design point-of-view; (iii) identify additional experimentation needs to reduce the most critical uncertainties; and (iv) establish acceptable levels of accuracy for property prediction models employed.