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Determination of the Uncertainty Bounds of a Continuous Distillation Code: Effect of Input Variability and Model Uncertainty

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Abstract

In this work, the effect of input variability and model uncertainty on the distillate composition of a continuous distillation tower is studied. To do that, we developed a stationary distillation code by combining mass and energy balance equations with a liquid-vapor equilibrium model and tray efficiency correlations. Feed and model uncertainties were modeled by using normal and uniform distributions respectively. A Monte Carlo propagation method was used to determine the upper and lower uncertainty margins of the distillate composition. The results of the application to a methanol-water distillation showed that the model uncertainty is as high as that of the feed variability. The information can be useful for the robust design of distillation towers.

Keywords: Uncertainty analysis; Monte Carlo method; Continuous distillation

1. Main text

The configuration and operation parameters of continuous distillation units are usually optimized for a specified feed and a required distillation composition. However, the control of the operation parameters is always necessary to counteract the effects of feed variability and other influent variables like external temperature. Current designs are made using process simulators whose calculations are based on thermodynamic models and correlations. The results predicted from these models and correlations can be inaccurate when the conditions differ from those that were used to fit the model parameters. A robust design of a distillation tower considering these two sources of uncertainty could reduce the number of control actions leading to a higher energetic efficiency.

In the paper, we study the effect of input variability and model uncertainty on the uncertainty margins of the distillate composition. The case of study is the distillation of a methanol-water mixture with a methanol fraction of z_F =0.36 in a distillation tower of 10 trays.

Due to the impracticability of modifying the parameters of a commercial code, we developed a multi-compartment model of a distillation tower. In the model, the mass and energy balance equations for the lumped

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compartments (condenser, reboiler and trays) are combined with a liquid-vapor equilibrium model (NRTL) and correlations to determine tray efficiency. The latter equations constituted the higher source of model uncertainty. To solve the equations, the procedure starts by guessing the vector x of compositions of the liquid streams. Given x, the flows of liquid and vapor of the different streams are obtained by using the balance equations for mass and energy and those of equilibrium and efficiency. Next, the calculation step yields to a new vector x obtained by using the balances of component in every compartment. An iterative procedure is applied to the calculation steps to achieve the convergence of x.

A Monte Carlo propagation method was used to study the effects of each source of uncertainty on the distillate fraction of methanol x_D. Doubly-truncated normal distributions with a coefficient of variation of 0.05 were considered to describe the statistical uncertainty of the feed related variables (flow, composition and enthalpy). The NRTL and tray efficiency correlation parameters were described by uniform distributions. All available experimental data were comprised between the model predictions for the lower and upper bounds of the uniform distributions. The criterion to determine the number of Monte Carlo runs was that the response variable was comprised between the upper and lower boundary margins with a probability of 95% and a confidence level of 99%. According to Wilks' formula (Wilks, 1941) the number of model runs was 181. To minimize computation time and facilitate convergence, all solutions generated during the Monte Carlo Method were saved to be used as initial guesses for the following runs.

A sensitivity analysis was also performed by correlating the response with every input variable (Hofer, 1999). This analysis yielded that the feed composition had much effect on the feed uncertainty than the flow or enthalpy as it was strongly correlated with x_D.

The results for different reflux ratios (Fig. 1) showed that the model uncertainty can be as high as that related to the feed variability. The global uncertainty, including input variability and model uncertainty, showed asymmetric distributions with a separation between upper bound and the average greater than the separation between average and lower bound. The separation between margins is not greatly affected by the reflux ratio.

The information obtained can be useful for the robust design of distillation towers.

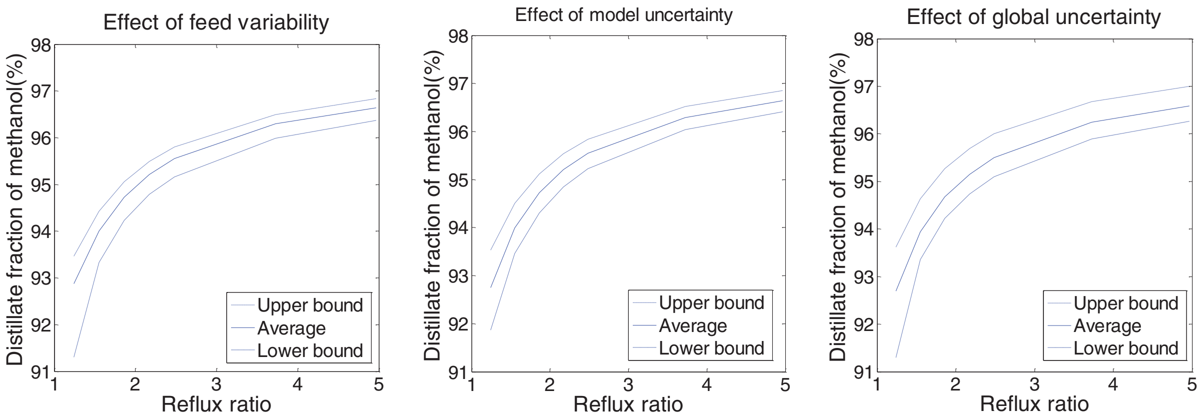

Figure 1. Uncertainty bounds for the distillate fraction of methanol for a probability of 95% as a function of the reflux ratio.

2. References

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