496c Improved Procedure for Estimating Process Design Reliability

Elim R. Myers and Colin S. Howat III

Chemical process designs are based on computations with uncertain parameters sets, e.g. phase equilibria, kinetics and feed. The parameter uncertainty leads to uncertainty in whether the process will meet constraints under normal operation, if built. The certainty that it will meet constraints is the process design reliability, usually expressed as a percentage. This reliability can be estimated using Conventional Monte Carlo simulation, or a derivative thereof, of the entire design. This is computationally expensive.

An alternative developed at the Kurata Thermodynamics Laboratory is Monte Carlo Integration of the n-constraints mapped onto the p-parameter space. This methodology geometrically interpolates among constraint boundary points to determine the fraction of parameter sets that fall within the interpolated boundary. Confidence in the reliability estimate is improved with increasing number of boundary points. This method is three to four orders of magnitude more computationally efficient compared to Conventional Monte Carlo. The significant computational effort in this method is tangentially interpolating among the boundary points to estimate the constraint boundary.

This paper presents a more efficient interpolation by searching in the statistically most significant direction. Boundary interpolation is connecting instead of tangential eliminating p-derivative calculations at each boundary point. This paper shows that the method, while potentially requiring more boundary points, is an order of magnitude more computationally efficient. Example problems discussed focus on multicomponent distillation.