Reliable Modeling and Optimization for Chemical Engineering Applications: Interval Analysis Approach

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Abstract

In many applications of interest in chemical engineering it is necessary to deal with nonlinear models of complex physical phenomena, on scales ranging from the macroscopic to the molecular. Frequently these are problems that require solving a nonlinear equation system and/or finding the global optimum of a nonconvex function. Thus, the reliability with which these computations can be done often an important issue. Interval analysis provides tools with which these reliability issues can be addressed, allowing such problems to be solved with complete certainty.

This presentation will focus on three types of applications: 1) Parameter estimation in modeling of phase equilibrium, including implications of using locally vs. globally optimal parameters in subsequent computations; 2) Nonlinear dynamics, in particular the location of equilibrium states and bifurcations of equilibria in ecosystem models used to assess the risk associated with the introduction of new chemicals into the environment; 3) Molecular modeling, with focus on transition state analysis of diffusion of a sorbate molecule in a zeolite.