Reliable Modeling Using Interval Analysis: Chemical Engineering Applications

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Chemical engineers often deal with nonlinear models of complex physical phenomena, on scales ranging from the macroscopic to the molecular. Frequently these nonlinear models occur in process engineering problems requiring nonlinear equation solving and/or optimization. The reliability with which these problems can be solved is often an important issue. For example, in process optimization a consistent issue concerning reliability is whether or not a global, as opposed to local, optimum has been achieved. In process modeling, especially with the use of highly nonlinear models, the issue of whether a solution is unique is of concern, and if no solution is found, of whether there actually exists a solution to the posed problem. For some problems, the model may have multiple solutions and all must be found, with no *a priori* knowledge of the number of solutions that exist. Methods based on interval analysis provide the power to solve these problems reliably, in fact with mathematical certainty.

In recent years, interval-Newton-based methods have begun to be used for the reliable solution of chemical engineering problems such as:

(1) phase stability analysis using excess Gibbs energy models (Stadtherr *et al.*, 1995; McKinnon *et al.*, 1996; Tessier *et al.*, 2000) and cubic equation of state models (Hua *et al.*, 1996, 1998),

(2) computation of homogeneous azeotropes (Maier *et al.*, 1998) and reactive azeotropes (Maier *et al.*, 2000),

(3) computation of mixture critical points (Stradi *et al.*, 2001),

(4) computation of solid-fluid equilibrium (Xu *et al.*, 2000) and

(5) parameter estimation in vapor-liquid equilibrium models (Gau *et al.*, 2000).

In each case, the interval methodology is used to deal rigorously with issues of multiple (or no) roots in nonlinear equation solving problems or issues of multiple local extrema in optimization problems.

In this presentation, the focus will be on some new applications of interval methods to solve nonlinear modeling and optimization problems in chemical engineering. Of particular interest are (1) some relatively large dimension problems (largest with 264 variables) arising from parameter estimation using the error-in-variables approach and (2) some molecular-scale problems arising in density functional theory and in statistical associating fluid theory. Improvements in the methodology used to solve these problems will also be discussed.

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