INTERVAL ANALYSIS: APPLICATION TO CHEMICAL ENGINEERING DESIGN PROBLEMS

Interval analysis can provide valuable tools in several aspects of chemical process design, including steady-state process simulation and optimization, and the initial synthesis and screening of process alternatives. The discussion below highlights the use of interval analysis in these areas. for a general description of problems and issues in chemical engineering design, see [9] and [8].

Process Simulation. Process simulators are used to compute the performance of a chemical process given its design (the *process simulation* problem), or to compute a design that meets given performance specifications (the *process design* problem). In either case, the central problem in steady-state process simulation is the solution of an $n \times n$ system of nonlinear algebraic equations $\mathbf{f}(\mathbf{x}) = \mathbf{0}$, where n may be very large (hundreds of thousands) and the equation system represents a mathematical model of the process, including material and energy balances, thermodynamic equilibrium relationships, and other equations needed to describe the process.

For solving the process model, Newton and quasi-Newton methods are widely used, but may not reliably converge, especially since a good initial guess is often hard to obtain. To improve convergence in these circumstances, various approaches have been used. These include trust-region techniques, such the *dogleg method* [4], and *homotopy-continuation* methods (e.g., [10]).

An additional difficulty is that in process simulation there are invariably upper and lower bounds on the variables, $\mathbf{x}^L \le \mathbf{x} \le \mathbf{x}^U$, violation of which may cause some functions to become undefined. Bounds are often dealt with in an *ad hoc* manner involving truncation or reflection of the correction step. A more natural way of dealing with bounds is to use a mathematical programming approach (e.g., [1]), in which the bounds become an integral part of the problem. While a number of the techniques noted above demonstrate excellent global convergence properties in practice, none offer a rigorous mathematical guarantee of convergence.

A further difficulty in solving the nonlinear equation systems arising in process simulation is that they may have multiple solutions. With the exception of homotopy-based methods, none of the techniques mentioned above are designed for finding multiple solutions when they exist. While in practice homotopy-based methods are frequently able to locate all solutions to a problem, they offer no guarantee that all solutions have been found, except in special cases.

All of the difficulties noted above, namely the lack of good initial guesses, the presence of variable bounds, and the possibility of multiple solutions, can be dealt with using interval analysis. For example, `R. E. Swaney and C. E. Wilhelm` [11] use a technique, based on repeated solution of linear programs, which, through the use of bounds generated using interval analysis within a branch and bound framework, provides rigorous global convergence to a solution of the process model.

`C. A. Schnepper and M. A. Stadtherr` [6] use an *interval Newton* approach. This can rigorously enclose any and all solutions to the process model, and is essentially initialization independent, since it requires only initial intervals for the variables, and some of these bounds may be specified as part of the problem. Both serial and parallel implementations are described in [6], and provision is made for efficient handling of sparse matrices. Several example problems were successfully solved, ranging in size from 3 to 177 variables, including problems with multiple solutions. Performance on the larger problems was unpredictable, with two problems of over one hundred variables being solved very efficiently, even with very large initial bounds

process simulation
process design
dogleg method
homotopy-continuation
interval Newton

on the variables, but one problem of 50 variables being unsolvable due to excessive computation time. However, for this 50-variable problem, once smaller, more intelligently chosen (using knowledge of boiling points and critical temperatures) initial intervals were used, the problem was easily and efficiently solved.

Process Optimization. Perhaps the most natural formulation for a process design problem is as an optimization problem. The process simulation problem is then viewed as an optimization problem with zero degrees of freedom. A typical process optimization problem features a nonlinear objective function, nonlinear equality constraints (the process model), nonlinear inequality constraints, and upper and lower bounds on variables. Frequently these nonlinear programming problems are nonconvex as well, prompting interest in global optimization techniques to deal with the potential for multiple extrema.

Several approaches to global optimization in process engineering have been proposed, including both deterministic and nondeterministic methods. Among the deterministic techniques used are branch and bound, cutting plane, primal-dual decomposition, and interval analysis. The work of `R. Vaidyanathan and M. El-Halwagi` [5] provides a good example of the use of interval analysis in this context. This is an interval branch-and-bound approach that is guaranteed to yield the global solution. The procedure is accelerated by using a "distrust region" method for eliminating infeasible portions of the search space and by use of local methods for some purposes.

`R. P. Byrne and I. D. L. Bogle` [3] and `R. P. Byrne` [2] also use an interval branch-and-bound approach, but treat the interval lower bounding process as a convex programming problem. In [2] it is also shown how this interval-based approach can be applied in the context of modular process optimization software. Since modular software predominates commercially, this work is of particular interest.

Process Synthesis. Before the process simulation and optimization problems discussed above can be formulated, it is necessary to synthesize and screen process alternatives. These provide the base case problems for later process simulation and optimization studies. When there is uncertainty in design specifications, or when the design specification covers a range of values, then interval analysis can be a particularly useful tool in *process synthesis*.

For example, `B. W. Schug and M. J. Realff` [7] describe a problem involving the processing of high level nuclear waste. In this problem, the waste to be processed is characterized by intervals of composition, as are the requirements for a stable glass product. In [7], an interval propagation scheme that exploits the structure of the problem and a simple process model is developed, and it is demonstrated how to use this to screen process alternatives and to infer other knowledge about the process design.

Conclusion. Interval analysis provides tools that can be used to solve phase simulation problems with complete reliability, providing a method that can guarantee with mathematical and computational certainty that the correct result is found, and thus eliminating computational problems that are encountered with conventional techniques. The method is essentially initialization independent, deals with variable bounds naturally, and also guarantees the enclosure of multiple solutions if present. In process optimization, similar guarantees can also be provided that the global extremum has been found. There are many other problems in chemical process design, for instance in many aspects of process synthesis, that likewise are amenable to solution using this powerful approach.

process synthesis

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Mark A. Stadtherr
Department of Chemical Engineering
University of Notre Dame
Notre Dame, Indiana 46556
USA
E-mail address: markst@nd.edu

AMS 1991 Subject Classification: 65C20, 65G10, 90C90, 65H20.

Key words and phrases: interval analysis, process design, process simulation, process synthesis, process optimization.