Application of Interval Methods to Chemical Engineering Problems

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The need of reliably solving large-scale system of nonlinear equations often arises in the everyday practice of chemical engineering. The following difficulties can occur when performing these calculations with standard methods. (a) It remains unknown whether the problem is indeed infeasible or just the initial points were poor if the iteration fails after several attempts due to divergence or oscillation. (b) It is hard to prove non-trivial infeasibility of a problem. Such a proof is usually done by exploring the feasibility region with approximate models, if a theoretical methodology exists at all. (c) Even if the iteration stops without a warning, the obtained result can be completely wrong due to the finite internal representation of floating point numbers and / or inappropriately chosen stopping criteria. (d) Professional simulators can return one solution at a time without indicating possible existence of other solutions. As a consequence, finding multiple solutions / proving uniqueness of a solution requires making a troublesome case study. These difficulties (a)-(d) are known to occur when computing the steady states of azeotropic distillation (especially heterogeneous azeotropic distillation) and reactive distillation columns.

All of the difficulties listed above can be overcome by interval methods. The main disadvantage of interval root-finding methods is the combinatorial explosion because these algorithms involve exhaustive search. In general, their applicability is limited to small problems (say 10 variables and equations). The goal of the research was to identify the bottlenecks and to improve the overall efficiency of the computations. A new general purpose root-finding algorithm has been proposed [1, 2, 5, 6, 7, 8] based on affine arithmetic and linear programming. The implementation is written in C++ programming language. The method is fairly general, and is applicable to a wide variety of engineering problems.

To the author's best knowledge, computation of distillation columns with interval methods had not been considered earlier in the literature. The MESH equations of an extractive distillation column are successfully solved with the proposed method in acceptable computation time [1, 5, 6, 7]. The convergence is guaranteed, initial estimation of the column profile is not needed. If no solution exists than this information is provided by the solver as a result. It is possible to give (redundant) interval specifications.

Reliably computing multiple steady states of distillation columns is crucial to their design, simulation, control and operation. Even ideal two-product distillation columns can have multiple steady states (output multiplicity). The proposed method finds all of them in one run, without any user intervention [5, 6, 7].

Numerical difficulties associated with the determination of minimal detectable differences in general ANOVA designs (involves computation of the noncentral-F distribution) raise the overriding importance of correct values with guaranteed accuracy. A new and easy to implement self-verifying algorithm is presented for the computation of intervals containing the true values with mathematical rigor if the degree of freedom of the denominator of the F test statistic is even. The proposed algorithm makes it possible to systematically study the accuracy of existing scalar algorithms in an automated manner. Numerical examples are presented [3, 4, 9, 10, 11].

Publications on the subject of the dissertation

Refereed articles

[1] **A. Baharev**, T. Achterberg, E. Rév; *Computation of an extractive distillation column with affine arithmetic*; AIChE Journal, *in press* (*IF: 1.607*)

[2] **A. Baharev**, E. Rév; *Reliable Computation of Equilibrium Cascades with Affine Arithmetic*; AIChE Journal, 2008, **54** (7), 1782–1797 (*IF: 1.607*)

[3] **A. Baharev**, E. Rév; *Rigorous enclosures of minimal detectable differences for general ANOVA models*; submitted to Reliable Computing

[4] **A. Baharev**, S. Kemény; *On the computation of the noncentral F and noncentral beta distribution*; Statistics and Computing, 2008, **18** (3), 333–340 (*IF: 1.136*)

Presentations

[5] **Baharev A.**; *Intervallum módszerek alkalmazása vegyészmérnöki számításokban*; az MTA Vegyipari Műveleti Munkabizottságának, a Műszaki Kémiai Komplex Bizottságának és a Magyar Kémikusok Egyesülete Műszaki Kémiai Szakosztályának együttes ülése; Veszprém, 2009. április 23.

[6] **Baharev A.**; *Intervallum módszerek alkalmazása vegyészmérnöki számításokban*; Oláh György Doktori Iskola VI. konferenciája, Budapest, 2009. február 4.

[7] **A. Baharev**, E. Rév; *Comparing inclusion techniques on chemical engineering problems*; 13th GAMM - IMACS International Symposium on Scientific Computing, Computer Arithmetic, and Verified Numerical Computations SCAN'2008; El Paso, Texas, USA, Sept 29 - Oct 3, 2008; pp. 17–18.

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Presentations not related to the dissertation

[12] **Baharev A.**, Frits E., Lelkes Z., Rév E.; *Megbízható fázisegyensúlyi számítások*; Műszaki Kémiai Napok'06, Veszprém, 2006. április 25–27. 288–289. o.

[13] **A. Baharev**, E. R. Frits, Cs. Stéger, Z. Lelkes, E. Rév; *Application of interval arithmetics for exploring feasibility region of extractive distillation*; 10. International Workshop on Chemical Engineering Mathematics; Budapest, Hungary, Aug 18–20, 2005

[14] E. R. Frits, **A. Baharev**, Z. Lelkes, M. Markót, Z. Fonyó, E. Rév, T. Csendes; *Feasibility Study by interval arithmetics: Application of interval arithmetics for exploring feasibilty of extractive distillation variants*; International Workshop on Global Optimization; Almería, Spain, Sep 18–22, 2005 (G05); in Proceedings of the International Workshop on Global Optimization; Ed. I. García et al., pp. 103–108, 2005

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