Optimization-Based Design of Reaction-Separation Systems

G. Sand[1], S. Barkmann[1], and S. Engell[1]

Abstract: A current trend in the chemical industries is to intensify processes by integrating reaction and separation operations. The conceptual design of integrated reaction-separation systems constitutes non-convex optimization problems of large scale which can be addressed by engineered mixed-integer non-linear programming (MINLP) techniques. In this presentation, non-standard modeling and solution techniques are presented and their potentials and the limitations are discussed by means of three test problems.

The modeling framework is a superstructure of identical building blocks with two phases which optionally provide reactive and separating functionality. The existence of an optional building block in the optimal structure is represented by a binary variable. The numerical solution of standard models typically suffers from their combinatorial complexity in addition to singularities caused by zero streams in case of non-existing building blocks. The non-standard modeling techniques presented here comprise an *indivisible quantities approach* to avoid zero streams, a *minimal binary approach* to reduce the dimension of the discrete subspace, and a *continuous reformulation approach* to eliminate discrete variables.

The non-convex constraints, originating e. g. from reaction kinetics, phase equilibria and cost models, give rise to multiple local optima of significantly different qualities. Two initialization strategies, namely *expert's initialization* and *evolutionary initialization*, are compared to *trivial initialization* with respect to their solution effort and their solution quality.

The modeling and solution techniques were tested for the conceptual design of two reactive distillation systems (production of methyl tertiary butyl ether and production of methyl acetate) and one reactive extraction system (production of mono-telomere). For reactive distillation, the *indivisible quantities approach* and the *continuous reformulation approach* turned out to be efficient, in contrast to the *minimal binary approach*. For well studied problems, the *expert's initialization* leads to high quality solutions, whereby otherwise the *evolutionary initialization* is the method of choice at the price of an increase of the computational cost by factors 10^2 to 10^3. A study of reactive extraction exhibited that an immediate transfer of the approach developed for reactive distillation is not possible: In contrast to the latter case, the number of phases in each building block is not fixed but variable, and its computation is a non-trivial task.

[1] Process Control Laboratory
Department of Biochemical and Chemical Engineering
Universität Dortmund
44221 Dortmund, Germany
{*g.sand*|*s.barkmann*|*s.engell*}*@bci.uni-dortmund.de*