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An efficient solution method for the MINLP optimization of chemical processes

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Abstract

Process synthesis often involves the solution of large nonlinear discrete-continuous optimization problems, which are usually formulated as mixed-integer nonlinear programming (MINLP) or generalized disjunctive programming (GDP) problems and solved with MINLP solvers. This paper presents an efficient solution method for these problems named successive relaxed MINLP (SR-MINLP), where the model formulations are reformulated to contain only continuous variables. The discrete decisions are relaxed and successively tightened in a sequential solution procedure to facilitate convergence and to obtain local optima of good quality. The solution method is illustrated by a simple numerical example as well as a large and complex example from process synthesis.

Keywords: MINLP, continuous reformulation, distillation design

1. Introduction

Chemical processes often demand enormous capital as well as operating costs. Designing the optimal, i.e. most cost effective process can save significant amounts of financial resources. In practice, this task is often approached by tedious, repetitive simulation studies of the process. In addition to the tedious nature of this procedure, the simulation studies suffer the drawback that good solutions for the process design are often overlooked. Rigorous economic optimization of chemical processes, however, is capable of identifying local optimal solutions by applying mathematical programming methods, which are often stated as MINLP [1] or GDP problems [2]. The discrete-continuous nature of these optimization problems stems from the discrete design variables (e.g. number of units, number of column trays) and the continuous design and operating variables (e.g. vessel sizes, flowrates, energy duties).

MINLP problems are usually solved with mixed-integer algorithms including Outer Approximation iterations or Branch and Bound, where a tree evaluation in the integer search space is performed. When applied to large and non-convex process design problems like the economic optimization of distillation processes, these MINLP procedures often suffer from robustness problems, require long computation times and often identify optima of low quality.

A discrete-continuous optimization problem can be reformulated as a purely continuous optimization problem and solved with reliable NLP solvers by replacing the discrete variables with continuous variables. Stein et al. suggested adding non-convex special constraints to the continuously reformulated optimization problem in order to force integer decisions on the continuously relaxed decision variables. It has been observed, however, that the solution of a continuously reformulated problem with these non-convex special constraints is highly dependable on good initial guesses due to the non-convex nature of the formulation. To overcome this drawback of continuous reformulations we propose in this work to relax and subsequently tighten the special constraints in a sequential solution procedure. In the resulting optimization formulation called successive relaxed MINLP (SR-MINLP), a succession of NLP problems with decreasing bounds is solved.

The solution procedure is illustrated by two case studies. The first case study is a simple example to illustrate the SR-MINLP solution procedure. The second case study covers a complex MINLP optimization problem from process design: the economic optimization of an extractive distillation process in terms of capital and operating costs. The optimization results obtained with the SR-MINLP procedure are compared to results obtained with established MINLP solvers applied to the discrete-continuous or the continuously reformulated MINLP problems without relaxation.

2. Methodology

Nonlinear optimization problems involving discrete and continuous variables can be formulated as MINLP problems or as generalized disjunctive programs (GDP). The general MINLP problem formulation is as follows:

$$\begin{aligned} &\min_{x,y} f(x,y), \\ &s.t. \quad g(x,y) \le 0, \quad x \in X, y \in Y, \end{aligned} \tag{1}$$

where x are continuous variables and y are integer variables. A discrete-continuous optimization problem can also be formulated as a GDP problem composed of disjunctive regions in the following form:

$$\min_{x,Y} \Phi(x) + \sum_{k\in K} b_k$$
$$\text{s.t.} \quad g(x) \le 0, \qquad \bigvee_{i\in D_k} \begin{bmatrix} Y_{i,k} \\ h_{i,k}(x) \le 0, \\ b_k = \gamma_{i,k}, \end{bmatrix}, \quad k \in K, \tag{2}$$
$$D_k = \{1,2,...,n_k\}, \quad K = \{1,2,...,m\}, \quad \Omega(Y) = \text{True}, \quad Y_{i,k} \in \{\text{True}, \text{False}\}.$$

Comments on the notation of the GDP problem can be found in [1], [2] and [3]. GDP problems can be solved with logical solvers that are capable of handling logic constraints. However, the development of such solvers has not yet progressed sufficiently. Therefore GDP problems are usually reformulated as MINLP problems and solved with available MINLP solvers.

Recently, different continuous reformulations (CR) of MINLP/GDP problems have been proposed. Stein et al. [3] introduced the continuous reformulation of GDP problems with tailored big-M constraints, where all discrete decisions are represented by exact continuous variables. The discrete decisions are enforced by special constraints which force the continuous variables to discrete values. The problem formulation reads as [3]:

$$\min_{x,Y} \Phi(x) + \sum_{k\in K} b_k$$
$$\text{s.t.} \quad g(x) \le 0, \qquad h_{i,k}(x) \le M_{i,k}\left(\sum_{j\in D_k\setminus\{i\}} y_{j,k}\right),$$
$$-M_{i,k}\left(\sum_{j\in D_k\setminus\{i\}} y_{\text{j,k}}\right) \le b_k - \gamma_{i,k} \le M_{i,k}\left(\sum_{j\in D_k\setminus\{i\}} y_{\text{j,k}}\right), \tag{3}$$
$$Ay \le a, \quad \sum_{i\in D_k} y_{i,k} \ge 1, \quad k \in K, \qquad \varphi_{\text{FB}}\left(y_{i,k}, \sum_{j\in D_k\setminus\{i\}} y_{j,k}\right) = 0, \quad i \in D_k, k \in K.$$

Equation φ_{FB} is the so-called Fischer-Burmeister function that constitutes the special constraints which force the integer decisions on the continuously relaxed decision variables $y_{i,k}$:

$$y_{i,k} + \sum_{j\in D_k\setminus\{i\}} y_{j,k} - \sqrt{{y_{i,k}}^2 + \sum_{j\in D_k\setminus\{i\}} {y_{j,k}}^2} = 0. \tag{4}$$

Similarly, MINLP problems can be reformulated by relaxing the integer variables and introducing the Fischer-Burmeister function or comparable special

constraints. However, continuous reformulations employing non-convex Fischer-Burmeister or comparable functions should only be employed if the original MINLP/GDP optimization problem is non-convex itself. The solution of a continuously reformulated problem can be attained with a reliable NLP solver like SNOPT and, thus, the iterations or the tree search of MINLP solvers like Outer Approximation and Branch and Bound, respectively, are avoided. As a consequence, large nonlinear optimization problems can be solved substantially faster after continuous reformulation. Still, the continuous reformulation suffers from the drawback that the quality of the local optimal solution is highly dependable on the specified initial values to start the solution procedure due to the distinct non-convexity.
To counter this drawback of the continuous reformulation we propose here to relax the Fischer-Burmeister according to

$$y_{i,k} + \sum_{j \in D_k \setminus \{i\}} y_{j,k} - \sqrt{{y_{i,k}}^2 + \sum_{j \in D_k \setminus \{i\}} {y_{j,k}}^2} - M_{\mathrm{FB}} \le 0 \tag{5}$$

and to subsequently tighten it again in a sequential solving procedure. The resulting so-called successive relaxed MINLP (SR-MINLP) is solved in a sequential solving procedure where the SR-MINLP problem is tightened with each step by reducing the value of the big-M-like parameters M_{FB}. In the succession of optimization steps M_{FB} takes on the values 0.5/0.2/0.1/0.05/0. Note that the successive steps are suitably initialized by the previous step and therefore very short solution times are observed.

3. Case Studies

3.1. Simple illustrative example

In order to illustrate the solution procedure, the first case study is a simple GDP problem with one disjunction taken from Lee and Grossmann [5]:

$$\begin{aligned}
&\min_{x,Y} (x_1 - 3)^2 + (x_2 - 2)^2 + b \\
&\text{s.t.} \quad 0 \le x_i \le 8, \quad i = 1,2, \\
&\begin{bmatrix} Y_1 \\ (x_1)^2 + (x_2)^2 - 1 \le 0 \\ b = 2 \end{bmatrix} \vee \begin{bmatrix} Y_2 \\ (x_1 - 4)^2 + (x_2 - 1)^2 - 1 \le 0 \\ b = 1 \end{bmatrix} \vee \begin{bmatrix} Y_3 \\ (x_1 - 2)^2 + (x_2 - 4)^2 - 1 \le 0 \\ b = 3 \end{bmatrix}, \\
&Y_i \in \{\text{True, False}\}, \quad i = 1, 2, 3.
\end{aligned} \tag{6}$$

Lee and Grossmann [5] reformulate and solve the GDP as an MINLP and identify the global optimum of 1.172, since Eq. (6) is a convex optimization problem. Stein et al. [3] reformulate the problem according to Eq. (3). The introduction of Eq. (4) gives rise to additional non-convexities and as a consequence, only local optimal solutions are found depending on the specified initial guesses.

For the SR-MINLP solution, the Fischer-Burmeister constraints are relaxed (cf. Eq. (5)) and successively tightened as explained above. With these modifications to the continuous reformulation of Stein et al., the sequential solution procedure of the SR-MINLP returns the global optimal solution for any choice of initial guesses. The initial problem of the solution procedure with a fully relaxed Fischer-Burmeister equation is convex and returns a good initial point for the subsequent steps with tightened bounds.

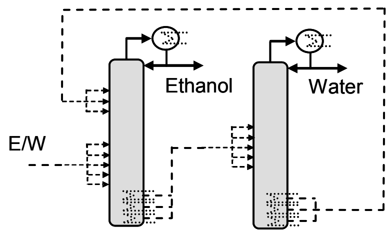

Fig. 1. Superstructure for the extractive distillation process.

3.2. Complex example from process design

The second case study covers a large and complex example from process design: the economic optimization of an extractive distillation process in terms of capital and operating costs for the separation of the homogeneous azeotropic mixture of water and ethanol with the help of glycol as the entrainer. The superstructure of the process optimization problem is sketched in figure 1. The process is fed with a mixture of 39.56 mol/s ethanol and 6.44 mol/s water from a bioethanol preconcentrator column. An ethanol purity greater than 0.9995 mol% is specified for the extractive column product. Water with a purity of 0.995 mol% is drawn of the recycling column and the entrainer glycol is recycled. Optimal integer values need to be determined for the number of column trays and for the locations of the feed streams, while optimal continuous values need to be found for the column energy duties and for the flow rates and compositions of the recycle and intermediate streams. The resulting nonlinear optimization problem is very complex due to its size, non-convexity and number of degrees of freedom. The arising optimization difficulties can be tackled by integrating the detailed optimization of distillation processes in a synthesis framework providing a favorable initialization [6] and by applying the SR-MINLP optimization described in Section 2.

The SR-MINLP column model formulations employed for this case study are based upon the formulations for single columns as presented by Kossack et al. [4]. The optimal values for the discrete variables in the process model are not necessarily located on integer values as it is the case for simple single columns [4]. Therefore relaxed Fischer-Burmeister functions as in Eq. (5) are added in order to force the continuously relaxed discrete variables to take on integer values in the solution. A performance chart of the considered solution methods is given in table 1. The SR-MINLP solution identifies a better local optimum and requires less CPU time than the MINLP solution of the same process model. The continuous reformulation without relaxation suffers from the significant dependence of the solution quality on the initial guess.

Table 1. Comparison of solution methods for the process optimization example.

	total annualized cost	CPU time
MINLP (Branch & Bound)	€ 1214501	897.5 s
MINLP (Outer Approximation)		did not converge
Continuous Reformulation	€ 1271429	80.3 s
SR-MINLP	€ 1209237	120.2 s

4. Summary and Conclusion

In this contribution, discrete-continuous optimization problems (MINLP/GDP) are solved by an efficient solution method based on continuous reformulations and a sequential solution procedure with tightened bounds (SR-MINLP). The tedious iterations or tree searches of conventional MINLP solution algorithms can be avoided by the SR-MINLP solution procedure since the solver can resort to reliable NLP algorithms. Two case studies are presented and it is shown that the SR-MINLP solution compares favorably to the MINLP solution and the continuous reformulation without relaxation. It is planned to apply the SR-MINLP optimization method for heterogeneous distillation and also for hybrid processes with different unit operations like membrane separation cascades or crystallization cascades in the near future.

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