A Decomposition-based MINLP Solution Method Using Piecewise Linear Relaxations

Pradeep K. Polisetty and Edward P. Gatzke[1]

Department of Chemical Engineering

University of South Carolina

Columbia, SC 29208

Submitted to ITOR, International Transactions on Operations Research

A rigorous decomposition-based approach for solution of nonseparable mixed-integer nonlinear programs involving factorable nonconvex functions is presented. The proposed algorithm consists of solving an alternating sequence of Relaxed Master Problems (a Mixed-Integer Linear Program) and nonlinear programming problems. The number of major iterations can be significantly decreased by use of piecewise linear relaxations of the nonconvex functions. The introduction of piecewise linear relaxations improves the lower bound on the problem but increases the number of constraints and binary variables in the Relaxed Master Problem. A sequence of valid nondecreasing lower bounds and upper bounds are generated by the algorithm that converge in a finite number of iterations. Numerical results are presented for example problems, illuminating the potential benefits of the proposed algorithm.

Keywords

Mixed integer nonlinear programming, decomposition algorithms, global solution, piecewise linear relaxations, deterministic nonconvex optimization.

[1] Author to whom correspondence should be addressed: gatzke@sc.edu

1 Introduction

Global optimization can be described as a procedure that attempts to find the alsolute best objective value that satisfies all conditions. Mathematical programming is an efficient method for optimization of various problems which are often quite difficult. Combinatorial optimization is a branch of optimization which includes a discrete search space. These problems are generally NP-hard and are often quite difficult to be solved. In many cases, these problems can be shown to exhibit combinatorial complexity which in the worst case requires examination of all binary realizations and essentially requires the total enumeration of the binary space. A very general class of difficult optimization problems involving integer and continuous variables can be defined as:

$$
\begin{aligned}
& \min_{x,y} f(x,y) \\
\text{s.t.} \quad & \phi(x,y) = 0 \\
& g(x,y) \leq 0 \\
& x \in X \subset \mathbb{R}^n \\
& y \in Y = \{0,1\}^q
\end{aligned}
\tag{1}
$$

The solution of this problem requires one to determine the minimum of a real valued function f subject to constraints defined by vector-valued functions g and ϕ in the continuous-discrete (x-y) space with n continuous variables and q binary variables. Note that integer and discrete valued variables with given lower and upper bounds may be represented by sets of binary variables [17]. Additionally, equality constraints can be represented by two inequality constraints without loss of generality. Problems of this type are generally termed Mixed-Integer Nonlinear Programming (MINLP) problems. Although the presence of binary variables makes the problem nonconvex, in many cases the individual functions f, ϕ_i, or g_i may also be nonconvex. Nonconvexities in continuous only nonlinear programming problems gives rise to multiple local optima and classical descent or hill-climbing methods may only yield local solutions which are far from being globally optimal. Traditional approaches of nonlinear programming have only been very successful in determining local optimal solutions because of the nonconvexities in the optimization problems and hence these approaches are still inadequate. The solution procedure for problems involving discrete and continuous variables can be even more complicated as the problem space involves a combinatorial number of discrete points i.e., the set of feasible solutions is discrete as some of the variables are restricted to take only discrete values. Finding global optima of nonconvex mixed integer nonlinear optimization problems has been an important paradigm for recent optimization researchers. In this work, we considered global optimization of nonseparable and factorable nonconvex nonlinear programming problems. The name *factorable function* denotes that these functions are recursive combinations of sums and products of univariate functions. Additionally, a function is separable if it can be transformed to a product of different functions where each new function will depend on only one of the original variables. Most functions of several variables used in nonlinear optimization are factorable and can easily brought into separable form.

Many industrial and process design problems such as heat exchanger network synthesis problem [45] and reactor network design problems [30] have some kinds of nonlinearities when posed as optimization problems. For instance, in order to attain better designs for existing or new processes in the area of process synthesis in chemical engineering it is often required to solve nonconvex mixed integer nonlinear optimization problems. Applications of MINLP have also emerged in the area of Design [22, 23], Production scheduling [34], and Planning of batch/continuous processes in chemical engineering [43]. Other applications include parameter estimation in molecular mechanics force fields and yield optimization of biochemical systems [44].

Global optimization algorithms can be primarily classified into two categories: Stochastic [38, 13] vs. Deterministic [40, 24]. Stochastic global optimization methods randomly search for global optimum over the domain of interest and typically rely on statistics and probabilistic arguments to prove convergence to the global solution. Additionally, convergence cannot be accurately proved. The advantage of these methods is that they don't need a specific structure for the problem being solved and may help when the problems involve uncertainty or randomness, or when the problem does not have a suitable algebraic formulation. Other disadvantage is that they often cannot handle highly constrained optimization problems and do not offer bounds on the solution. Some of these methods include: Simulated annealing [36, 10, 12], Tableau search [20], and Genetic algorithms [21]. As opposed to stochastic methods, deterministic global optimization methods can rigorously guarantee optimal solutions within an ϵ tolerance, where this tolerance is the difference between the objective function value of the true global optimum point and that of the solution obtained. Deterministic global optimization techniques can explicitly handle large constrained optimization problems, and therefore are often favorable compared to stochastic techniques. These techniques however require specific mathematical structure and hence can only be applied to specific problems in order to obtain global solutions. Identifying global solutions with arbitrary accuracy however presents significant advantages and challenges. These algorithms proceed by rigorously reducing the feasible space until the global solution has been found with prescribed accuracy. Converging sequences of valid upper and lower bounds are generated which approach the global solution from above and below. The rigorous generation of bounds on the optimal solution is a significant part of deterministic global optimization and this usually requires generation of convex function relaxations to nonconvex expressions.

Several methods for solving MINLP problems have been proposed in the past. These methods include Branch-and-Bound [16, 33, 24], Generalized Benders Decomposition GBD [6, 19], and Outer-Approximation algorithms [14]. Recently, improved interior point methods have been developed to solve MINLP problems [8]. Most of the existing techniques for solving MINLP problems require assumptions on the types of allowable constraint or objective functions to determine global solution. Recently, an Outer-Approximation based algorithm for separable nonconvex MINLP problems was developed by Kesavan et al [28, 27]. This algorithm depends on generation of relaxations to the original problem and consists of solving an alternating sequence of Mixed-Integer Linear Programming (MILP) Problems and two Non Linear Programming (NLP) problems. The shortcoming with this technique is that it may often result in total enumeration of the binary space due to poor relaxations. The goal of the current work is to examine algorithms for solution of nonconvex MINLP problems using improved relaxation techniques.

Numerous methods [2, 31, 41] have been proposed to construct convex relaxations of general nonconvex functions. The reformulation method of McCormick [31, 39, 9] converts the original factorable nonconvex nonlinear algebraic functions into an equivalent form by the introduction of new variables and constraints. The reformulated problem contains only linear and simple nonlinear constraints. The convex relaxations for the simpler nonlinear constraints can be constructed using the convex and concave envelopes that are known for many simple algebraic functions. The αBB method [2, 1] also generates convex relaxations for general twice-differentiable constrained nonlinear problems. One advantage of this method as compared to the basic reformulation technique is that αBB does not require introduction of new variables. The αBB method requires the determination of bounds on the minimum eigenvalues of the Hessian of the nonconvex functions. The Hybrid relaxation method [18] combines both basic reformulation and αBB methods. This method may be advantageous in some cases where one of the above mentioned methods fails to generate a tight convex relaxation for the original NLP. Convex linear relaxations can also be generated by using the linearization strategy of Tawarmalani and Sahinidis [41]. This method generates a convex nonlinear relaxation for the original factorable nonlinear problem. This nonlinear convex relaxation is further relaxed using multiple linearizations based on outer approximation at multiple points. The feasible space resulting from these outer approximations gives a convex linear relaxation of the original nonlinear problem. The bound on the relaxed problem is found by the solution of the resulting convex Linear Programming (LP) problem.

Global optimization algorithms when used with the existing relaxation techniques may take a large amount of time to converge to the global solution. In this work, a method using a MILP-based piecewise linear relaxation technique is used for generating relaxations to nonconvex expressions. Using McCormick's [31] reformulation method together with the propositional logic constraints [5, 4, 42], the original nonlinear problem is relaxed to a MILP problem. The solution to this MILP problem gives the lower bound on the original problem. This method is similar to previous decomposition methods [7] but uses solution of the upper bounding NLP problem by spatial branch-and-bound or branch-and-reduce. This method appears to be advantageous in cases where the above mentioned relaxation methods fail to generate tight function relaxations, with the reservation that it requires the solution to a nonconvex MILP problem. The MILP relaxation can provide a tight lower bound making use of existing robust MILP solution methods. The quality of this lower bound can be modified by changing the number of piecewise linear regions used in the lower bounding MILP problem. The availability of robust Mixed Integer Programming (MIP) solvers like CPLEX 8.1 [26] and IBM OSL [25] may justify the use of this particular technique in many cases for solving nonconvex nonlinear problems. Solution of the MILP lower bounding problem is often quite rapid due to well-developed branch-and-cut methods.

A rigorous decomposition-based approach for solutions of nonseparable factorable MINLP problems is presented. The method proceeds by iteratively solving an sequence of MILPs and NLPs. A piecewise linear relaxation technique is used for generation of relaxations to nonconvex expressions. The use of piecewise linear relaxations improves the lower bound on the problem but can increase the problem complexity of the lower bounding MILP. A sequence of valid non-decreasing lower bounds and upper bounds is generated by the algorithm that converge in a finite number of iterations. A convergence proof is provided.

2 Problem Description and Reformulation

The class of nonconvex MINLPs considered in the present work conform to the following formulation.

$$
\mathrm{P} = \begin{cases} \min\limits_{x,y} f(x,y) & \\ \text{s.t. } g(x,y) & \leq \quad 0 \\ x \in X \subset \mathbb{R}^m & \\ y \in Y = \{0,1\}^q & \end{cases} \tag{2}
$$

where $f : X \times Y \to \mathbb{R}$ and $g : X \times Z \to \mathbb{R}^p$ with $Y \subset Z = \mathbb{R}^q$, with f and g_i are continuous and possibly nonconvex. The problem as defined by equation 2 will be referred to as P hereafter. These assumptions are sufficient to guarantee that either a minimum exists or the problem is infeasible. Without loss of generality, the problem can be rewritten as:

$$
\mathrm{P1} = \begin{cases} \min\limits_{x,y} x_0 & \\ \text{s.t. } \acute{g}(x,y) & \leq \quad 0 \\ x \in X \subset \mathbb{R}^m & \\ y \in Y = \{0,1\}^q & \end{cases} \tag{3}
$$

Here, $\acute{g}$ now includes a new variable and an additional constraint and in the form $f(x,y) - x_0 \leq 0$. Assuming that all g_i are factorable, new variables and constraints can be used to simplify the problem nonlinearity. Some of the new variables are defined by linear constraints, while some variables are defined by simple nonlinear equality constraints involving two or three variables. See 2.2 for details on reformulation of nonlinear expressions. The new problem can be written in the form:

$$
\text{P2} = \begin{cases} \min\limits_{x,y} x_0 \\ \text{s.t. } A_1[x^T\, y^T w^T]^T \leq B_1 \\ A_2[x^T\, y^T w^T]^T = B_2 \\ w - h(x,y,w) = 0 \\ x \in X \subset \mathbb{R}^m \\ y \in Y = \{0,1\}^q \\ w \in W \subset \mathbb{R}^{l+n} \end{cases} \tag{4}
$$

Here, $h : X \times Y \times W \to \mathbb{R}^n$ define the n new nonlinear variables and l linear equality constraints are introduced to define the new linear variables. Bounds are derived on w based on the original bounds for x and y using interval analysis [32]. The problem as defined by equation 4 will be referred to as P2 hereafter. Obviously, this problem is nonconvex, as any nonlinear equality constraint requires that the resulting mathematical programming problem be nonconvex. It is assumed that Problems P, P1, and P2 are equivalent.

This reformulation is useful in that convex underestimating and concave lower bounding functions can readily be determined for each individual nonlinear function h_i. As a result, a convex nonlinear problem can be formulated as follows:

$$
\text{P3} = \begin{cases} \min\limits_{x,y} x_0 \\ \text{s.t. } A_1[x^T\, y^T w^T]^T \leq B_1 \\ A_2[x^T\, y^T w^T]^T = B_2 \\ \check{h}(x,y,w) \leq w \leq \hat{h}(x,y,w) \\ x \in X \subset \mathbb{R}^m \\ y \in Y = \{0,1\}^q \\ w \in W \subset \mathbb{R}^{l+n} \end{cases} \tag{5}
$$

Here, $\check{h}_i$ is a convex underestimating function for h_i and $\hat{h}_i$ is a concave overestimating function for h_i. Note that many of the resulting under and overestimating functions are actually linear functions which result from the secants derived for convex or concave envelopes. Additionally, bilinear nonlinear terms result in four new linear inequality constraints for convex relaxation. Also note that problem P3 is still nonconvex, as $y \in \{0,1\}^q$. If the integrality constraint for y were removed from problem P3, the solution of the resulting convex NLP would provide a lower bound on the solution of P, P1, and P2.

Problem P3 can be further relaxed by outer approximation of the nonlinear convex and concave constraint functions. This allows for all the constraints to be written as linear equations, resulting in a mixed integer linear program:

$$\text{P4} = \begin{cases} \min\limits_{x,y} x_0 & \\ \text{s.t. } A_1[x^T\, y^T w^T]^T \leq B_1 & \\ A_2[x^T\, y^T w^T]^T = B_2 & \\ A_3[x^T\, y^T w^T]^T \leq B_3 & \\ x \in X \subset \mathbb{R}^m & \\ y \in Y = \{0,1\}^q & \\ w \in W \subset \mathbb{R}^{l+n} & \end{cases} \tag{6}$$

Here, the constraints defined in A_3 are composed of the linear secant constraints from the relaxation of simple functions, the linear constraints appearing due to relaxation of bilinear terms, and linear constraints introduced due to linearization of convex nonlinear functions at multiple points. As bounds on all variables are known, linearization of the convex constraints may be performed at multiple locations, resulting in a tunable parameter that allows for improvement of the relaxation value. As additional linearizations are introduced, the solution of P4 should approach the solution of P3. Both P3 and P4 are valid relaxations of the original problem P.

2.1 Piecewise Linear Relaxations

In the previous section, the problem was relaxed based on convex and concave under and over estimating functions. The feasible space of problem P2 can alternatively be relaxed by introduction of propositional logic constraints. These logic constraints will allow for tight relaxation of nonconvex functions, but the new constraints will require additional binary variables.

A MILP-based piecewise linear relaxation technique can generate tighter relaxations as compared to those generated by LP-based and NLP-based relaxation methods. The problem space for the nonlinear function is divided into multiple regions using propositional logic constraints. Outer approximations of convex or concave nonlinear functions and secant under-estimates and over-estimates are then generated for each individual region, thereby converting the mixed integer nonlinear problem P3 into a mixed integer linear programming problem. Most of the constraints in this MILP problem are relaxed while enforcing only those constraints corresponding to the single region containing the solution.

The variable space for x is divided into S regions separated by $(S-1)$ boundaries. A binary variable b_i is introduced for each region resulting in S new binary variables. For the S regions, $2(S-1)$ propositional logic inequality constraints are then added to represent these regions. In this technique, b_1 is forced to a take a value of 1 if x is between x^l and s_1, where s_1 is the upper bound on the first region. The first region constraint is specified as follows:

$$-s_1 + x \leq M(1 - b_1)$$

The regions 2 through $(S-1)$ are specified with the following constraints:

$$\begin{aligned} s_1 - x + \delta &\leq M(1 - b_2) \\ -s_2 + x &\leq M(1 - b_2) \\ s_2 - x + \delta &\leq M(1 - b_3) \\ -s_3 + x &\leq M(1 - b_3) \\ &\vdots \end{aligned} \tag{7}$$

where δ is a small value used to ensure that the value of the variable x does not end up at the boundaries separating the regions. The final region constraint is specified as follows:

$$s_{(S-1)} - x + \delta \leq M(1 - b_S)$$

Since only a single region can contain the solution, an equality constraint is added to ensure that solution lies in only one region.

$$\sum_{i=1}^{S} b_i = 1 \tag{8}$$

Based on these propositional logic constraints and the constraint shown in Equation 8, if the value of the variable x is smaller than s_1, the binary variable b_1 is forced to take value of 1. On the other hand, if a binary variable takes a value of zero, the respective constraint is relaxed as the right hand side takes a large value of M. The nonlinear expression is replaced by outer approximation constraints written for each region. Depending on the number of linearizations, O, used to outer approximate the nonlinear expression in each piecewise region, the linear over-estimate constraints for a concave nonlinear expression can be written as follows:

$$
\begin{aligned}
w \;\; \leq \;\; & f(x)|_{x=x^*_{i,j}} + \left.\frac{\partial f(x)}{\partial x}\right|_{x=x^*_{i,j}} (x - x^*_{i,j}) + \, M(1-b_i) \\
& \forall\, x^*_{i,j},\ where\ j = 1..O\ and\ \forall\, i = 1..S
\end{aligned}
$$

where $x^*_{i,j}$ are the linearization points, $f(x)$ is the nonlinear expression, and $\frac{\partial f(x)}{\partial x}$ is the gradient of the nonlinear expression. For each region, the nonlinear expression can be under estimated by a secant constraint written as follows:

$$
secant(f(x),\, x^L,\, x^U) \leq w + M(1-b_i) \qquad \forall\, i = 1...S
$$

where x^L, x^U are the lower and upper bounds for a particular region. Constraints corresponding to a convex nonlinear expression can be written similarly with a sign change. If the binary variable related to a particular region takes a value of 1, the corresponding linearization and secant constraints are enforced while relaxing the constraints corresponding to other regions. The final MILP-based piecewise linear relaxation problem can be represented in a general form as follows:

$$
\text{P5} = \begin{cases}
\begin{aligned}
\min_{x,y,w,z} x_0 & \\
\text{s.t. } A_1[x^T\, y^T w^T]^T & \leq b_1 \\
A_2[x^T\, y^T w^T]^T & = b_2 \\
A_3[x^T\, y^T w^T]^T & \leq b_3 \\
A_4[x^T\, y^T w^T z^T]^T & \leq b_4 \\
x \in X \subset \mathbb{R}^m & \\
y \in Y = \{0,1\}^q & \\
z \in Y = \{0,1\}^r & \\
w \in W \subset \mathbb{R}^{l+n} &
\end{aligned}
\end{cases} \tag{9}
$$

Here, z are the binary variables introduced and $A_4\left[x^T y^T w^T z^T\right]^T \leq b_4$ are the linear constraints representing logic constraints, outer approximation constraints, and secant constraints for all Q regions.

2.2 Example Reformulation and Relaxation

The reformulation of the original MINLP problem (P) into an equivalent simpler MINLP problem (P2) is illustrated on an standard test problem taken from Handbook of Test Problems in Local and Global Optimization [15].

$$
\begin{aligned}
\min_{x,y} \quad & 2x_1 + 3x_2 + 1.5y_1 + 2y_2 - 0.5y_3 \\
1.25 \;=\; & x_1^2 + y_1 \\
3 \;=\; & x_2^{1.5} + 1.5y_2 \\
-1.6 \;\leq\; & -x_1 - y_1 \\
-3 \;\leq\; & -1.333x_2 - y_2 \\
0 \;\leq\; & y_1 + y_2 - y_3 \\
& 0 \leq x_1, x_2 \leq 10 \;, y \in \{0,1\}^3
\end{aligned}
$$

As mentioned earlier, the MINLP test problem which is of the form P is reformulated into an equivalent simpler form P2. New variables, x_0 for the objective function and $w_1$and w_2 for nonlinear terms are introduced resulting in a simple nonlinear MINLP problem shown below. It can be seen that bounds on these new variables are derived based on original bounds for x and y using interval analysis. The simplified nonlinear problem shown in Equation 10 is of the form P2.

$$
\begin{aligned}
\min_{x,y} \quad & x_0 \\
1.25 &= w_1 + y_1 \\
3 &= w_2 + 1.5y_2 \\
-1.6 &\leq -x_1 - y_1 \\
-3 &\leq -1.333x_2 - y_2 \\
0 &\leq y_1 + y_2 - y_3 \\
x_0 &= 2x_1 + 3x_2 + 1.5y_1 + 2y_2 - 0.5y_3 \\
w_1 &= x_1^2 \\
w_2 &= x_2^{1.5} \\
& 0 \leq x_1, x_2 \leq 10 \\
& 0 \leq w_1 \leq 100 \\
& 0 \leq w_2 \leq 31.6 \\
& y \in \{0,1\}^3
\end{aligned} \tag{10}
$$

The MILP-based piecewise linear relaxation technique is graphically illustrated on the nonlinear constraint $w_2 = x_2^{1.5}$ involved in the above problem. Here, w_2 is the new variable introduced during reformulation and 1.5 is a non-integer constant. The nonlinear expression is of the form $w = x^c$ with the secant under estimating constraint and outer approximation based over estimating constraints shown in Figure 1. In this example, the variable space for x is divided into 2 regions and 2 linearizations are derived for each region. Complex factorable nonlinear problems can be automatically reformulated using McCormick's method so that the final reformulated problem has expressions that involve only 2 or 3 variables. These simple expressions include bilinear terms xy, variable raised to constants x^c, where c can be non integer constant, even integer, odd integer, or negative integer. Other expressions include natural log of a variable $ln(x)$, exponential of a variable

$exp(x)$, $sin(x)$, $cos(x)$. In the case of bilinear terms, binary variables and logic constraints can be used for both variables. MILP-based piecewise linear relaxations can be developed to nonconvex problems involving these simple nonlinear terms.

xpowerc-examplemain-modified.eps

Figure 1: (a) Original nonlinear nonconvex constraint $w = x^c$. (b) Relaxation of $w = x^c$ using the secant under estimate. (c) Two outer approximation constraints over estimating the nonlinear expression resulting in linear constraints. (d) Two outer approximation constraints and a secant under estimate constraint for each region in the MILP-based piecewise relaxation problem.

3 MINLP Solution Algorithm

A decomposition-based deterministic global optimization algorithm for solutions of nonconvex MINLP problems is presented. As stated, this algorithm may often result in total enumeration of the binary space due to generation of poor relaxations. The advantage with the decomposition-based algorithm is that it may require fewer number of major iterations with the use of MILP-based piecewise linear relaxation technique.

The proposed algorithm iteratively solves an alternating sequence of Relaxed Master Problems (MILP) and nonlinear programming problems (NLPs). The use of piecewise linear relaxations improves the lower bound on the problem but increases the number of constraints and binary variables in the Relaxed Master Problem MILP. Tighter bounds on the variables can be obtained by performing a nonlinear presolve based on interval analysis prior to global search for the solution. After setting the initial upper and lower bounds on the problem, a Relaxed Master Problem P5 is solved to generate a valid lower bound to the solution of original MINLP problem. A nonconvex NLP problem is obtained by fixing the binary variables in the original problem P to the integer realization obtained from the solution of Relaxed MILP problem. This nonconvex NLP problem is then solved to global solution using Branch-and-Reduce [35] global optimization algorithm. As the algorithm proceeds, integer cuts [3] are added to the MILP lower bounding problem to ensure that previously examined integer realizations are excluded. The solution of the Relaxed MILP problem with added integer cuts yields a new integer realization and the iteration is repeated. A sequence of valid nondecreasing lower bounds and upper bounds are thus generated by the algorithm. These bounds converge in a finite number of iterations when the lower bound exceeds the upper bound by some ϵ tolerance.

The advantage of using MILP-based piecewise linear relaxation technique is that much tighter lower bounds are generated. The MILP algorithm branches on all original binary variables and the new binary variables introduced during reformulation using propositional logic. The MINLP algorithm terminates in fewer major iterations as the branching on continuous variables is significantly decreased as the decomposition-based MILP lower bound jumps from $y(k)$ to $y(k+1)$ solving global NLP for upper bound. Assuming the original binary variables are branch upon first with the new binary variables branched only after all original variables are specified, this technique is illustrated in the figure 2. Tighter lower bounds on the MINLP objective function can be derived with the reservation that one must find the solution of a more difficult Relaxed Master MILP problem. However, the availability of robust MILP solvers and the fewer iterations during MINLP algorithm may justify the use of this particular technique. The robustness of MILP solvers is due to various branch-and-cut cutting plane methods.

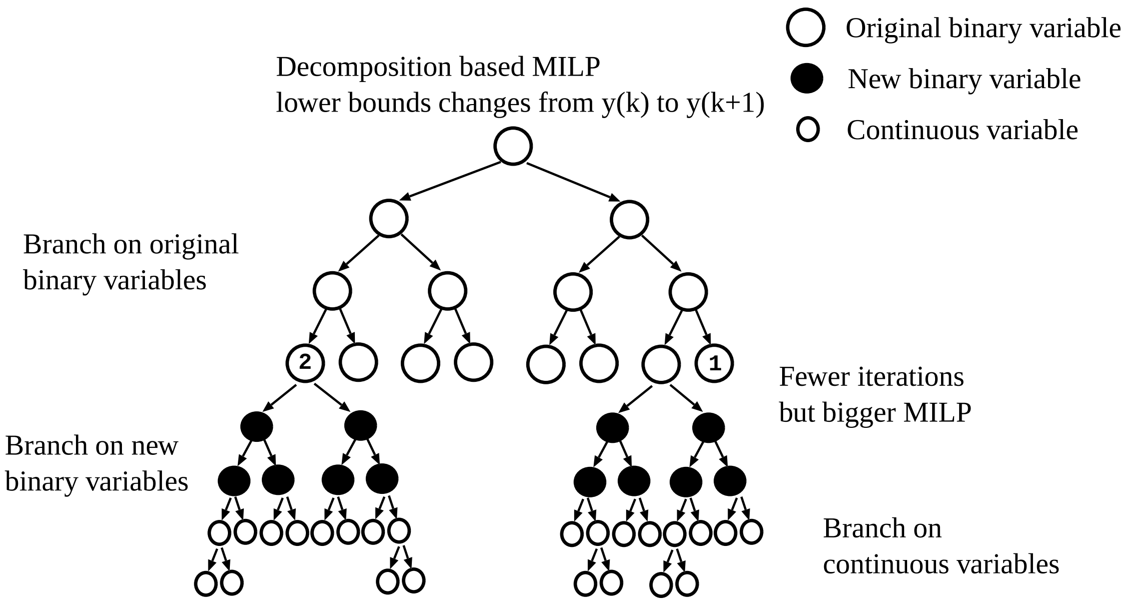

Figure 2: Illustration of variable branching in decomposition-based MILP lower bounding technique.

The proposed MILP-based piecewise linear relaxation technique and MINLP solution algorithm are implemented in Matlab® and is scheduled for distribution as an open source software package called Global Optimization Toolbox for Matlab (GLOBO). Several tools for performing variable bound contraction using interval analysis and optimization-based bound tightening [35] are included in the package. The decomposition-based MINLP algorithm is illustrated in the flow chart shown in Figure , and can be explained by the following pseudo code.

Algorithm 1 Pseudo code for decomposition-based MINLP algorithm.

Perform nonlinear presolve to tighten variable bounds based on interval analysis
Set UBD = ∞, LBD = $-\infty$, $k = 0$
Solve Relaxed MILP problem P5 for $y(k)$ and LBD
If (Infeasible)
  LBD =∞
END If
While LBD $<$ UBD - ϵ
  Solve nonconvex NLP problem with y fixed to $y(k)$ to get an upper bound $U(k)$
  If (Feasible and $U(k)$ $<$UBD)
    UBD = $U(k)$
  END If
  Add integer cuts to Relaxed MILP problem to exclude $y(k)$
  $k = k + 1$
  Solve Relaxed MILP problem P5 for $y(k)$ and LBD
  If (Infeasible)
    LBD = ∞
  END If
END While

decomp-minlp.eps

Figure 3: Flow chart for Decomposition-based MINLP algorithm.

Theorem 1. The MINLP solution algorithm terminates in a finite number of steps with ϵ convergence providing an optimal solution to P or terminates indicating that P is infeasible.

Proof.

First it is shown that the algorithm terminates in a finite number of steps. The set $\mathbf{Y} = \{0,1\}^Q$ contains all possible combinations of the original binary variables in the original MINLP problem. Since the set $\mathbf{Y}$ is finite, the integer cuts added to the Relaxed Master Problem MILP are finite. Therefore the MINLP solution algorithm terminates in a finite number of major iterations.

Second it is shown that the algorithm terminates with an ϵ convergence providing an optimal solution to the problem if P is feasible or else indicate that the problem P is infeasible.

Upon termination at iteration k, we have f^*, x^*, y^* as the solution to original MINLP problem P where $f^*$is the optimal solution objective function, x^* is the continuous variable solution, and y^* is the binary variable solution. The theorem is proved by contradiction that no better solution to the MINLP problem exists other than the best solution found so far. For this, assume that an improved solution does exist with $f^{'} < f^*$, and $y^{'} \in \mathbf{Y} \backslash Y_K$ where Y_K is the set of all points in the binary variable space that includes all the integer cuts added to the Relaxed MILP problem $P5$ at the termination step, step K. The MILP relaxation problem $P5$ with integer cuts excluding some set Y_K is a lower bound on the MINLP problem P that excludes those Y_K. From the above statement we have:

$$P5(Y_K) \leq P(\mathbf{Y} \backslash Y_K) \tag{11}$$

The Algorithm terminates when the MILP lower bound exceeds the best upper bound found i.e. $P5(Y_K) \geq NLP(y^*)$. As it was assumed that $y^{'}$ is an improved solution compared to y^*, we have

$$P5(Y_K) \geq NLP(y^*) \geq NLP(y^{'}) \tag{12}$$

But from Equation 11 we have $P5(Y_K) \leq P(\mathbf{Y} \backslash Y_K)$ and since NLP with fixed $y^{'}$ is an upper bound on MINLP problem P, we have $P(Y \backslash Y_K) \leq NLP(y^{'})$. This leads to

$$P5(Y_K) \leq P(Y \backslash Y_K) \leq NLP(y^{'}) \tag{13}$$

Equation12 contradicts Equation 13 thereby disproving our assumption that the overall problem P has a improved solution y' compared to the best solution y found so far. This proves that the MINLP algorithm terminates providing an optimal solution to P when the problem P is feasible.

If P is infeasible, the MILP lower bound may or may not be feasible. All nonconvex NLP problems with fixed y must be infeasible. The algorithm never updates the upper bound on the problem and terminates indicating that P is infeasible.

□

4 Computational Results

The decomposition-based MINLP algorithm is implemented on several standard global optimization test problems. Computational results are presented for three simple test problems taken from Chapter 12 of [15] and one larger scale problem. The MINLP solution algorithm is implemented in Matlab® by taking advantage of the Matlab's solver "fmincon" to determine feasible local solutions. At each major iteration, nonconvex NLP problems are guaranteed to global solution using Branch-and-Reduce based global optimization algorithm. CPLEX 8.1 is used for solution of MILP problems. The proposed algorithm is implemted in Matlab 6.5 on a hyperthreaded 3.20 GHz Intel Pentium(R) 4 CPU with 1 Gbyte memory running a Debian-based Linux installation using a SMP version of the 2.6.6 kernel.

As mentioned earlier, the quality of the lower bound can be modified by changing the number of piecewise linear regions used in the lower bounding MILP problem. Simple test problems can be solved quickly, so only 1 piecewise linear region is used during lower bound generation which is equivalent to LP-based relaxation. However, for the large scale problem, the algorithm requires large amount of time to converge to the global solution when traditional relaxation techniques are used. For this, more number of piecewise regions are used to demonstrate the potential benefit of MILP-based piecewise linear relaxation technique. Computational results for these test problems are shown in Table 1. For these simple problems, the nonconvex NLP problems obtained by fixing the binary variables are solved at the root node of the Branch-and-Reduce method. The number of major iterations, upper bound, and average total solution time are presented for each problem.

Problem 1.

This test problem was initially presented in [29].

$$\begin{aligned}
\min_{x,y} \quad & 2x_1 + 3x_2 + 1.5y_1 + 2y_2 - 0.5y_3 \\
1.25 \;=\; & x_1^2 + y_1 \\
3 \;=\; & x_2^{1.5} + 1.5y_2 \\
-1.6 \;\leq\; & -x_1 - y_1 \\
-3 \;\leq\; & -1.333x_2 - y_2 \\
0 \;\leq\; & y_1 + y_2 - y_3 \\
& 0 \leq x_1, x_2 \leq 10, \; y \in \{0,1\}^3
\end{aligned}$$

The global solution to this problem is attained at $x = (1.12, 1.31)^T$, $y = (0, 1, 1)^T$ with an objective function value of 7.667.

Problem 2.

This problem was presented in Pörn et al. (1997).

$$\begin{aligned}
\min_{x,y} \quad & 7x_1 + 10x_2 \\
24 \leq \; & -x_1^{1.2}x_2^{1.7} + 7x_1 + 9x_2 \\
-5 \leq \; & x_1 + 2x_2 \\
-1 \leq \; & 3x_1 - x_2 \\
-11 \leq \; & -4x_1 + 3x_2 \\
0 = \; & -x_1 + y_1 + 2y_2 + 4y_3 \\
0 = \; & -x_2 + y_4 + 2y_5 + y_6 \\
& 1 \leq x_1,\ x_2 \leq 5,\ \ y \in \{0,1\}^6
\end{aligned}$$

The minimum objective function value for Problem 2 is 31 attained at $x = (3,1)$, $y = (1,1,0,1,0,0)$. For Problem 3, the global minimum is 17 at $x = (4,1),\ \ y = (1,0,0)$.

Problem 3.

This problem is taken from [27].

$$\begin{aligned}
\min_{x,y} \quad & -5x_1 + 3x_2 \\
-39 \leq \; & -2x_2^2 + 2x_2^{0.5} + 2x_1^{0.5}x_2^2 - 11x_2 - 8x_1 \\
-3 \leq \; & -x_1 + x_2 \\
-24 \leq \; & -3x_1 - 2x_2 \\
0 = \; & -x_2 + y_1 + 2y_2 + 4y_3 \\
& (1,\ 1) \leq x_1,\ x_2 \leq (10,\ 6) \\
& y \in \{0,1\}^3
\end{aligned}$$

Problem	1	2	3
Continuous Variables	2	2	2
Binary Variables	3	6	3
Average Solution Time (secs)	1.78	0.33	1.44
Major Iterations in MINLP Solution Algorithm	1	1	1

Table 1: Computational results for 3 simple MINLP test problems.

Problem 4:

A highly nonconvex nonlinear problem is formulated in order to test the robustness of the proposed MINLP algorithm. The objective is to minimize x_2 subject to some large number of parabola constraints. The problem is then converted to a MINLP problem by assigning a binary variable associated to each parabola subject to its presence in the problem formulation. For test purposes, the problem is formulated to contain 60 parabolas. The objective is to determine how the global minimum value of x_2 changes as some parabolas are removed. In the problem formulation, a_i, b_i, and c_i are the coefficients associated with each parabola, M is a large number used to formulate the conditional constraints using propositional logic [5, 4, 42], and T is the number of parabolas to be removed.

$$
\begin{aligned}
\min_{x_1, x_2} \quad & x_2 \\
a_i(x_1 - y_i)^2 + c_i \quad & \leq \quad x_2 + M\, y_i \quad \forall i \\
\sum_{i=1,..,n} y_i \quad & = \quad T \\
0 \leq \quad & x_i \quad \leq 1 \\
y_i \quad & \in \quad \{0, 1\}^q
\end{aligned}
$$

Computational results are presented in Table 2. For the parabolas removed, the maximum number of possible combinations of the parabolas that can be removed, the upper bounds, and number of major iterations during MINLP solution algorithm are shown. The best binary realization that resulted in global minimum are also presented. Results are presented for the case of 16 piecewise linear regions during MILP lower bound generation. The proposed decomposition-based MINLP algorithm is then compared with BARON [37, 41], a Branch-and Reduce Optimization Navigator for mixed integer nonlinear programming problems. For computational and performace comparison purpose, the number of Branch and Reduce (BaR) iterations and the solution times are presented in Table 2. It can be noted that the newly proposed deomposition based MINLP algorithm, when implemented on the 60 parabola test problem, converged to the global solution requiring significantly fewer iterations and in a considerably short amount of time when compared to BARON. Proposed MINLP algorithm and BARON are both implemented using $1e^{-9}$ absolute termination tolerance. It was also observed that upon termination, the optimality gap was considerably smaller when the proposed MINLP algorithm is used.

Parabolas Removed	Possible Combinations	Upper Bound	MINLP Algorithm		BARON		Binary Realization
			Major Iterations	Time (secs)	BaR Iterations	Time (secs)	
0	1	7.24	2	3.43	19	0.42	
1	60	6.72	6	18.44	104	3.12	4
2	1770	5.96	3	7.47	568	6.24	4,53
4	487635	4.32	3	11.37	3897	57.55	45,47,51,,58
8	255×10^7	-1.32	3	19.42	17506	247.63	9,19,26,29,45,47,51,58

Table 2: Computational results for 60 parabola MINLP problem.

Results for the problems optimized when $0, 2$ and 4 parabola constraints are removed from the overall problem are graphically illustrated in Figure 3. In Figure 3, the curve represented by (a) is the nonconvex nonlinear objective function. The horizontal straight line represented by (b) is the global minimum for each problem. Optimal combinations of parabolas that are to be removed to get to the global solution are represented by (c). It can be noticed that as additional parabola constraints are removed from the original problem, the global minimum moves in the decreasing x_2 direction.

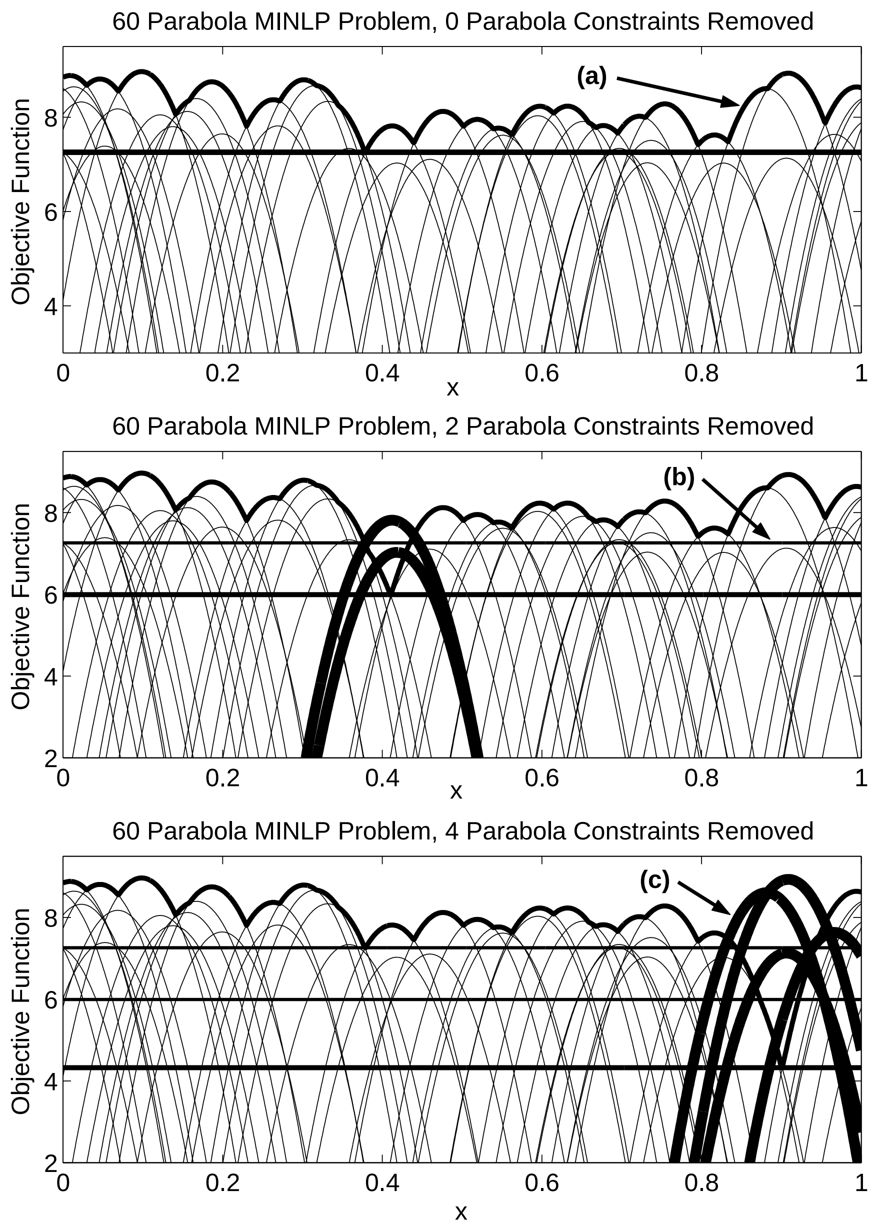

Figure 4: Graphical illustration of the results for 60 parabola MINLP problem. (a) Nonconvex objective function and the global solution when 0 parabola constraints are removed. (b) Parabolas that are removed and the improved global solution when 2 parabola constraints are removed. (c) Parabolas that are removed and the improved global solution when 4 parabola constraints are removed.

5 Conclusions

Numerous industrial and engineering design problems can be modeled as mixed integer nonlinear programming (MINLP) problems. The goal of this work is to develop a general purpose optimization algorithm to solve nonseparable factorable nonconvex MINLP problems. Convergence speed of the proposed decomposition-based MINLP algorithm can be significantly improved by generating tighter bounds on the objective function value. This task can be accomplished by the use of newly proposed MILP-based piecewise linear relaxation technique. Computational results justify and demonstrate the potential benefits of MILP-based relaxation techniques.

Acknowledgements

The authors would like to acknowledge financial support from the National Science Foundation under Grant No. 0238663. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the National Science Foundation. Additional support and collaboration was provided by DOE Sandia National Laboratories Computer Science Research Institute. The authors would also like to aknowledge NEOS server [11] for providing access to BARON.

References

[1] C. S. Adjiman, I. P. Androulakis, C. D. Maranas, and C. A. Floudas. A Global Optimization Method, α BB, for Process Design. *Comput. Chem. Eng.*, 20:S419–S424, 1996.

[2] C. S. Adjiman, S. Dalliwig, C. A. Floudas, and A. Neumaier. A Global Optimization Method, αBB, for General Twice-Differentiable Constrained NLPs - I Theoretical Advances. *Comput. Chem. Eng.*, 22(9):1137–1158, 1998.

[3] E. Balas and R. Jeroslow. Canonical Cuts on the Unit Hypercube. *SIAM J. Appl. Math*, 23:61–79, 1972.

[4] A. Bemporad and M. Morari. Predictive Control of Constrained Hybrid Systems. In *International Symposium on Nonlinear Model Predictive Control*, pages 108–127, Ascona, Switzerland, 1998.

[5] A. Bemporad and M. Morari. Control of Systems Integrating Logic, Dynamics, and Constraints. *Automatica*, 35:407–427, 1999.

[6] J. F. Benders. Partitioning Procedures for Solving Mixed-Variables Programming Problems. *Numer. Math.*, 4:238, 1962.

[7] M. L. Bergamini, P. Aguirre, and I Grossmann. Logic-based outer approximation for globally optimal synthesis of process networks. *Comput. Chem. Eng.*, 29:1914–1933, 2005.

[8] B. Borchers and J. E. Mitchell. An improved branch and bound algorithm for mixed integer nonlinear programs. *Comput. and Operations Research*, 21(4):359–367, 1994.

[9] R. P. Byrne and I. D. L. Bogle. Global optimisation of constrained non-convex programs using reformulation and interval analysis. *Comput. Chem. Eng.*, 23:1341–1350, 1999.

[10] O. Canton. Solving Scheduling Problems By Simulated Annealing. *SIAM J. Control Optim.*, 36(5):1539–1575, 1998.

[11] J. Czyzyk, M. Mesnier, and J. Moré. The NEOS Server. *IEEE Journal on Computational Science and Engineering*, 5:68–75, 1998.

[12] A. Dekkers and E. Aarts. Global Optimization and Simulated Annealing. *Mathematical Programming*, 50:367–393, 1991.

[13] M. A. H. Dempster. Introduction to Stochastic Programming. chapter Stochastic Programming, pages 3–62. New York: Academic Press, 1980.

[14] M. A. Duran and I. E. Grossmann. An Outer-Approximation Algorithm for a Class of Mixed-Integer Nonlinear Programs. *Mathematical Programming*, 36:307–339, 1986.

[15] C. A. Floudas *et. al*. *Handbook of Test Problems in Local Global Optimization*. Kluwer Academic Publishers, 1999.

[16] J. E. Falk and R. M. Soland. An Algorithm for Separable Nonconvex Programming Problems. *Management Science*, 15(9):550–569, 1969.

[17] C. A. Floudas. *Nonlinear and Mixed-Integer Optimization: Fundamentals and Applications*. Oxford UP, 1995.

[18] E. P. Gatzke, J. E. Tolsma, and P. I. Barton. Construction of Convex Function Relaxations Using Automated Code Generation Techniques. *Optimization and Engineering*, 3(3):305–326, 2002.

[19] A. M. Geoffrion. Generalized Benders Decomposition. *Journal of Optimization Theory and Applications*, 10:237–262, 1972.

[20] F. Glover. Tabu search part 1. *ORSA journal on Computing*, 1:190–206, 1989.

[21] D. E. Goldberg. *Genetic Algorithms in Search, Optimization, and Machine Learning*. Addison-Wesley, 1999.

[22] I. E. Grossmann, I. Quesada, R. Ramon, and V. T. Voudouris. Mixed-Integer optimization techniques for the design and scheduling of batch processes. In *Proc. of NATO Advanced Study Institute on Batch Process Systems Engineering*, 1992.

[23] I. E. Grossmann and R. W. H. Sargent. Optimal design of multipurpose chemical plants. *I and EC Proc. Des. Dev.*, 18(2):343, 1979.

[24] R. Horst and H. Tuy. *Global Optimization: Deterministic Approaches*. Springer-Verlag, Berlin, second edition, 1993.

[25] IBM-OSL. Optimization Solutions and Library Linear Programming Solutions. Technical report, I. B. M., 1997.

[26] ILOG. *ILOG CPLEX 8.1: User's Manual*. Mountain View, CA, July 2002.

[27] P. Kesavan, R. J. Allgor, E. P. Gatzke, and P. I. Barton. Outer Approximation algorithms for separable nonconvex mixed-integer nonlinearprograms. *Math. Program., Ser.A*, 100:517–535, May 2004.

[28] P. Kesavan and P. I. Barton. Decomposition Algorithms for Nonconvex Mixed-Integer Nonlinear Programs. *Fifth International Conference on Foundations of Computer-aided Process Design, Breckenridge, CO. AIChE Symposium Series*, 96:323–325, 2000.

[29] Gary R. Kocis and Ignacio E. Grossmann. Global Optimization of Nonconvex Mixed-Integer Nonlinear Programming (MINLP) Problems in Process Synthesis. *Industrial & Engineering Chemistry Research*, 1988.

[30] M. Manousiouthakis and D. Sourlas. A global optimization approach to rationally constrained rational programming. *Chem. Engng. Commun.*, 115:127–147, 1992.

[31] G. P. McCormick. Computability of Global Solutions to Factorable Nonconvex Programs: Part I - Convex Underestimating Problems. *Mathematical Programming*, 10:147–175, 1976.

[32] R. E. Moore. *Methods and Applications of Interval Analysis*. SIAM, Philadelphia, 1979.

[33] I. Quesada and I. E. Grossmann. Global optimization algorithm for heat exchanger networks. *Industrial and Engineering Chemistry Research*, 32:487–499, 1993.

[34] G. V. Reklaitis. Perspectives on scheduling and planning process operations. In *Proc. 4th. Int. Symp. on Process Systems Engineering*, page 3.2.1, Montreal, Canada, 1991.

[35] H. S. Ryoo and N. V. Sahinidis. Global Optimization of Nonconvex NLPS and MINLPs with Application to Process Design. *Comput. Chem. Eng.*, 19(5):551–566, 1995.

[36] S. Kirkpatrick, C. D. Gelatt, and M. P. Vecchi. Optimization by simulated annealing. *Computer Science/Engineering Technology*, 220:671–680, 1983.

[37] N. V. Sahinidis and M. Tawarmalani. BARON 7.2.5: Global Optimization of Mixed-Integer Nonlinear Programs, User's manual, 2005.

[38] F. Schoen. Stochastic Techniques for Global Optimization : A Survey of Recent Advances . *Journal of Global Optimization*, 1:207–228, 1991.

[39] E. M. B. Smith. *On the Optimal Design of Continuous Processes*. PhD thesis, Imperial College, London, 1996.

[40] E. M. B. Smith and C. C. Pantelides. A symbolic reformulation/spatial branch-and-bound algorithm for the global optimisation of nonconvex MINLPs. *Computers and Chemical Engineering*, 23:457–478, 1999.

[41] M. Tawarmalani and N. V. Sahinidis. Global optimization of mixed-integer nonlinear programs: A theoretical and computational study. *Mathematical Programming*, 99(3):563–591, 2004.

[42] M. L. Tyler and M. Morari. Propositional Logic in Control and Monitoring Problems. *Automatica*, 35:565–582, 1999.

[43] J. Vaselenak, I. E. Grossmann, and A. W. Westerberg. An embedding formulation for the optimal scheduling and design of multiproduct batch plants. *I and EC Res.*, 26(1):139, 1987.

[44] E. O. Voit. *Computational Analysis of Biochemical Systems : A Practical Guide for Biochemists and Molecular Biologists*. Cambridge University Press, Cambridge, UK, 2000.

[45] T. F. Yee and I. E. Grossmann. Simultaneous Optimization Models for Heat Integration - II. Heat Exchanger Network Synthesis. *Comput. Chem. Eng.*, 14(10):1165–1184, 1990.