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Global Solution Approach for a Nonconvex MINLP Problem in Product Portfolio Optimization

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Abstract. The rigorous and efficient determination of the global solution of a nonconvex MINLP problem arising from product portfolio optimization introduced by Kallrath (2003) is addressed. The objective of the optimization problem is to determine the optimal number and capacity of reactors satisfying the demand and leading to a minimal total cost. Based on the model developed by Kallrath (2003), an improved formulation is proposed, which consists of a concave objective function and linear constraints with binary and continuous variables. A variety of techniques are developed to tighten the model and accelerate the convergence to the optimal solution. A customized branch and bound approach that exploits the special mathematical structure is proposed to solve the model to global optimality. Computational results for two case studies are presented. In both case studies, the global solutions are obtained and proved optimal very efficiently in contrast to available commercial MINLP solvers.

Key words: Branch and bound, Concave objective function, Global optimization, Mixed-integer nonlinear programming (MINLP), Piece-wise linear underestimator, Portfolio optimization

1. Introduction

The modeling of decision making in many processes, such as the design of chemical plants, often leads to nonconvex mixed-integer nonlinear programming (MINLP) problems. The solution of this class of problems is very challenging due to the presence of both the integer variables and the nonconvexities. A number of approaches have been proposed for the solution of such problems within the branch and bound framework. For example, Adjiman et al. (2000) introduced a powerful theoretical and algorithmic framework based on the αBB global optimization approach for twice-differentiable nonlinear programming (NLP) problems (Adjiman et al., 1998). Adjiman et al. (2000) developed two broadly applicable algorithms for the solution of nonconvex MINLPs: a special structure mixed-integer αBB algorithm (SMIM-αBB) for problems with general nonconvexities in the continuous variables and restricted participation of the binary variables, and a general structure mixed-integer αBB algorithm (GMIN-αBB) for the broader class of problems whose continuous relaxations are twice-differentiable. Westerlund et al. (1998) proposed a new theoretical and algorithmic approach, the extended cutting plane algorithm, for addressing problems with pseudoconvex functions. Ryoo and Sahinidis (1996) developed a standard branch-and-reduce algorithm, in which they introduced domain reduction through feasibility and optimality tests. Smith and Pantelides (1999) introduced a reformulation/spatial branch-and-bound algorithm for mathematical models that feature factorable continuous functions and binary variables. For a comprehensive discussion of the theoretical, algorithmic, and application related issues for global optimization problems that include mixed-integer nonlinear optimization models, interested readers are referred to Horst and Tuy (1996) and Floudas (2000).

In this work, we address the global solution of a nonconvex mixed-integer nonlinear programming (MINLP) problem arising from product portfolio optimization. The problem and related data are taken from Kallrath (2003). This nonlinear nonconvex portfolio optimization problem contains a design problem (determining the number and sizes of chemical reactors) coupled with an assignment problem (assigning products to reactors). Kallrath (2003) developed a nonconvex MINLP model featuring concave terms in the objective function and trilinear products in the constraints. Kallrath (2003) attempted to address this problem using two types of approaches: (i) a mixed-integer linear programming (MILP) representation with equivalent linear constraints and an approximate objective function; and (ii) two commercial MINLP solvers, including a local solver, SBB, and a global solver, BARON. The former approach was able to generate good solutions, but essentially only solved an approximation of the original problem and could neither estimate nor reduce the gap between the obtained approximate solutions and the real optimal ones. While in the latter approaches, both solvers employed performed very poorly due to weak lower bounds. They required a substantial amount of computational time for a small case study and could not find the optimal solution within many CPU hours for a large case study (see Kallrath, 2003).

In this paper we present an improved formulation and a customized branch and bound approach to address this portfolio optimization problem, which is able to solve it to global optimality rigorously and efficiently. The rest of this paper is organized as follows. Section 2 presents the problem of interest. Section 3 contains an improved mathematical model based on the one developed in Kallrath (2003) and proposes a global optimization framework. Section 4 describes in detail the global solutions of two case studies and compares the proposed approach with previous ones, followed by concluding remarks in Section 5.

2. Problem Description

Taken from Kallrath (2003), the portfolio optimization problem of interest is as follows. A business unit operating a number of batch reactors wants to analyze the dependence of investment and fixed costs on given demand spectra. In this paper we analyze two different scenarios: one includes a relatively large number of products (i.e., about 40 products) and the other involves a "*lean* assortment" with fewer products (i.e., about 20 products).

The analysis should determine cost minimal solutions. In addition to the costs, the following detailed results are expected:

- the number of reactors required and the number of batches per reactor;
- the volumes of the reactors;
- which batches are produced on a certain reactor;
- the utilization rates of the reactors;
- surplus production with respect to the demand.

The solution defines the optimal production configuration, and, in a second step, will help to perform product portfolio analysis.

The production configuration is subject to the following constraints:

1. The demand for 20 and 40 products, specified per week and per product, needs to be satisfied.
2. All products are subject to shelflife limits. Actually, the products can be stored for about one week; if they are properly cooled they can survive a few more days.
3. All products are produced in batches of 6 h.
4. The feasible volumes of the reactors are in the range between 20 and $250\,m^3$.
5. The filling degree or utilization rate needs to be at least 40%.

For each reactor, the fixed cost and the investment cost are known. Regarding the fixed costs, we should note that one person can control two reactors. The investment cost is given by a nonlinear concave function which relate the cost to the volume of the reactor. It is sufficient to consider investment costs which are qualitatively correct. The most important structural feature is that the investment-cost-versus-reactor-volume function is concave. Storage tanks are not included in our model and costs related to the production process and the storage tanks are not considered.

The following input data determine the size of the problem:

- the potential number of the reactors is between 2 and 4;
- the number of products is in the range between 20 and 40;

– the maximal number of batches per reactors is 28, which results from the number of hours available per week (168).

3. Mathematical Model

Based on the model in Kallrath (2003), an improved mathematical formulation is developed and will be discussed in detail as follows.

3.1. BASIC FORMULATION

First, we define the following indices, sets, and parameters:

Indices and sets

$p \in P$ products
$r \in R$ reactors

Parameters

Costs

C_r^F [kEuro/week] fixed cost of reactor r; 2.45 for all reactors
C_r^I [kEuro] investment or depreciation cost per m^3 for reactor r per week; 0.97 for all reactors

Capacities and other production data

C_r^T [hours] time capacity of reactor r; usually 168 h (full week)
T_p^P [hours] time required to produce one batch of product p; 6 for all products and all reactors

Demand data

D_p [m^3] demand for product p per week; varies between 2 and 15,000
S surplus production allowed relative to the demand; 1 for all products

Reactor data

V_r^{L} [m^3] lower limit on the reactor volume if reactor r is active; 20 for all reactors
V_r^{u} [m^3] upper limit on the reactor volume if reactor r is active; 250 for all reactors
$F(U_r^{\mathrm{L}})$ lower limit on the utilization rates; 0.4 for all reactors

We introduce the following variables:

Variables

δ_r binary variable, selection of reactor r
v_r [m^3] reactor volume of reactor r
n_{rp} number of batches for product p in reactor r
p_{rp} [m^3] production of product p in reactor r

Based on this notation, the objective function and the constraints are formulated as follows:

Reactor volume bounds

$$V_r^{\mathrm{L}} \cdot \delta_r \leqslant v_r \leqslant V_r^{\mathrm{U}} \cdot \delta_r, \quad \forall r \in R \tag{1}$$

The reactor volume is bounded by the given limits if a reactor is selected.

Production limits

$$n_{rp} \cdot v_r \cdot F \leqslant p_{rp} \leqslant n_{rp} \cdot v_r, \quad \forall r \in R,\ p \in P \tag{2}$$

The amount of production of each product in each reactor is bounded by the upper and lower limits of filling degree. Note that by introducing variable p_{rp} to replace the trilinear product $n_{rp} \cdot f_{rp} \cdot v_r$ in the model of Kallrath (2003), the model now contains only bilinear products $n_{rp}v_r$ between an integer variable and a continuous variable, which can be further linearized (see detail in the next section).

Demand fulfillment

$$D_p \leqslant \sum_{r \in R} p_{rp} \leqslant (1+S)D_p, \quad \forall p \in P \tag{3}$$

The demand for each product needs to be satisfied; on the other hand, surplus production is only allowed within a given limit.

Reactor time

$$\sum_p n_{rp} \cdot T_p^P \leqslant c_r^T \cdot \delta_r, \quad \forall r \in R \tag{4}$$

The total time a reactor is used cannot exceed the available time.
Objective function: minimization of all costs

$$\min\ c^T := \sum_{r \in R} C_r^F \cdot \delta_r + \sum_{r \in R} \sqrt{C_r^I \cdot v_r} \tag{5}$$

The total cost consists of two parts. One is the fixed cost represented by the first term; the other is the investment cost, which depend nonlinearly on the volume of the reactors, as given by the second term. Note that the second term does not need to have the binary variables indicating the selection of the reactors because the reactor volume is enforced to be zero by constraints (1) if a reactor is not selected.

The following additional constraints proposed in Kallrath (2003) to improve the model are also included:

Breaking the symmetry of reactors

$$v_r \leqslant v_{r+1} \quad \forall r \in R,\ r \neq N^R \tag{6}$$

Total reactor volume requirement

$$28 \sum_{r \in R} v_r \geqslant \sum_{p \in P} D_p. \tag{7}$$

3.2. LINEAR TRANSFORMATION

Each integer variable n_{rp} can be represented by a set of binary variables as follows:

$$n_{rp} = \sum_{d \in D} n^B_{rpd} \cdot 2^d \tag{8}$$

where $d \in D$ is the dth digit of a binary number and n^B_{rpd} is a binary variable that determines the value of the dth digit of the binary representation of n_{rp}.

Constraints (2) consist of bilinear products between an integer variable and a continuous variable (i.e., $n_{rp} \cdot v_r$). The integer variables can be replaced by its binary representation (8), which leads to bilinear products between a binary variable and a continuous variable, $n^B_{rpd} \cdot v_r$. To transform the bilinear terms to a linear form, we introduce a set of auxiliary continuous variables, x_{rpd}, to replace the bilinear terms, and a set of additional linear constraints as follows (Floudas, 1995):

$$\begin{aligned} &v_r - v_r^{\mathrm{U}}(1 - n^B_{rpd}) \leqslant x_{rpd} \leqslant v_r - v_r^{\mathrm{L}}(1 - n^B_{rpd}) \\ &v_r^{\mathrm{L}} \cdot n^B_{rpd} \leqslant x_{rpd} \leqslant v_r^{\mathrm{U}} \cdot n^B_{rpd} \quad \forall r \in R, p \in P. \end{aligned} \tag{9}$$

Note that similar techniques were proposed in Kallrath (2003) to transform the trilinear products in their original model to equivalent linear forms.

3.3. FURTHER TIGHTENING OF THE MODEL

To reduce the computational efforts required to obtain the optimal solution, a number of additional constraints have been identified to tighten the mathematical model.

It is found that restricting the number of batches for each product in all of the reactors and/or in each reactor in a reasonably tight range, as represented by the following constraints, can tighten the model significantly.

$$N_p^{\mathrm{L}} \leqslant \sum_{r \in R} \sum_{d \in D} n^B_{rpd} \cdot 2^d \leqslant N_p^{\mathrm{U}}, \quad \forall p \in P \tag{10}$$

$$N_{rp}^{\mathrm{L}} \leqslant \sum_{d \in D} n^B_{rpd} \cdot 2^d \leqslant N_{rp}^{\mathrm{U}}, \quad p \in \forall P,\ r \in R \tag{11}$$

where N_p^{L} and N_p^{U} are the lower and upper bounds on the number of batches for product p, respectively; N_{rp}^{L}, and N_{rp}^{U}, are the lower and upper bounds on the number of batches for product p in reactor r, respectively.

When we derive the range for the number of batches of each product in each reactor, the following insight is used: to utilize the reactors as efficiently as possible, products with larger demands should be processed in the larger reactors as much as possible and the products with smaller demands should be processed in the smaller reactors. By ordering the product demands and assigning them to the reactors based on the above principle, much tighter ranges can be derived. However, it should be pointed out that this does not mean the larger demands should be handled only in the largest reactor since the demand may not be an integer number times the reactor volume and hence there may be a small amount which leads to usage of the smaller reactors.

Furthermore, it can happen that there are products with the same amount of demand. To eliminate the resulting degeneracy, we can break the symmetry as follows. Assume that products p and p' have the same amount of demand and p precedes p' in set P, and there are three reactors, then the following constraints are introduced:

$$n_{r1,p} \cdot 28^2 + n_{r2,p} \cdot 28 + n_{r3,p} \leqslant n_{r1,p'} \cdot 28^2 + n_{r2,p'} \cdot 28 + n_{r3,p'}. \tag{12}$$

By reducing the feasible region and cut off degenerate solutions, the above model-tightening techniques help to accelerate substantially the convergence to the optimal solution.

3.4. LOWER-BOUNDING PROBLEM AND BRANCH AND BOUND FRAMEWORK

It should be pointed out that the mathematical formulation described above leads to a nonconvex MINLP problem with the following characteristics:

(i) the objective function consists of univariate concave terms and a constant term;
(ii) all the constraints are linear.

A lower bounding problem can be constructed by underestimating the concave objective function with piecewise linear approximations (Floudas, 1995). As an example, consider the following three-piece linear approximation of $\sqrt{v}$ over the range of $\gamma_1 \leqslant v \leqslant \gamma_4$:

$$C(v) = \begin{cases} \alpha_1 + \beta_1 \cdot v, & \text{for } \gamma_1 \leqslant v \leqslant \gamma_2 \\ \alpha_2 + \beta_2 \cdot v, & \text{for } \gamma_2 \leqslant v \leqslant \gamma_3 \\ \alpha_3 + \beta_3 \cdot v, & \text{for } \gamma_3 \leqslant v \leqslant \gamma_4 \end{cases} \tag{13}$$

where

$$\alpha_1 = \sqrt{\gamma_1} - \beta_1 \cdot \gamma_1, \quad \beta_1 = \frac{\sqrt{\gamma_2} - \sqrt{\gamma_1}}{\gamma_2 - \gamma_1};$$

$$\alpha_2 = \sqrt{\gamma_2} - \beta_2 \cdot \gamma_2, \quad \beta_2 = \frac{\sqrt{\gamma_3} - \sqrt{\gamma_2}}{\gamma_3 - \gamma_2};$$

$$\alpha_3 = \sqrt{\gamma_3} - \beta_3 \cdot \gamma_3, \quad \beta_3 = \frac{\sqrt{\gamma_4} - \sqrt{\gamma_3}}{\gamma_4 - \gamma_3}.$$

We introduce binary variables y_1, y_2, y_3, each one associated with a segment of the variable range, and continuous variables v^1, v^2, v^3. Then the above piecewise linear function can be modeled by the following linear system:

$$\begin{cases} C(v) = (\alpha_1 \cdot y_1 + \beta_1 \cdot v^1) + (\alpha_2 \cdot y_2 + \beta_2 \cdot v^2) + (\alpha_3 \cdot y_3 + \beta_3 \cdot v^3) \\ v = v^1 + v^2 + v^3 \\ \gamma_1 \cdot y_1 \leqslant v^1 \leqslant \gamma_2 \cdot y_1 \\ \gamma_2 \cdot y_2 \leqslant v^2 \leqslant \gamma_3 \cdot y_2 \\ \gamma_3 \cdot y_3 \leqslant v^3 \leqslant \gamma_4 \cdot y_3 \\ y_1 + y_2 + y_3 = 1 \\ y_1, y_2, y_3 \text{ are binary variables.} \end{cases} \tag{14}$$

The resulting lower bounding problem is a mixed integer linear programming (MILP) problem which can be solved efficiently.

A branch and bound framework can then be used to solve for the global solution of the problem, which relies on the convergence between the lower bounds obtained by solving the lower bounding MILP problem and the upper bounds which are feasible solutions of the original MINLP problem (for more details of the branch and bound framework, see Floudas, 2000). Note that the constraints remain the same in the lower bounding problem and therefore any feasible solution obtained from the lower bounding problem is also a feasible solution of the original problem and the value of the objective function of the original problem, which can be obtained by simple function evaluation, provides a valid upper bound.

4. Computational Results of Specific Case Studies

Two different sets of demand data, taken from Kallrath (2003), are studied in this work. The data is given in Table 1. The mathematical models in this work are formulated with GAMS (Brooke et al., 1988) and the MILP problems are solved with CPLEX 7.0 (ILOG, Inc., 2000).

4.1. A SMALL CASE STUDY: SCENARIO 2

Two reactors are introduced and note that the bounds of the reactor volumes can be tightened based on the total demand and the time capacity. A total volume of $9860/28 = 352.14\,\text{m}^3$ is required, that is, $v_1 + v_2 \geqslant 352.14$. Because $v_2 \leqslant 250$, $v_1 \geqslant 102.14$; because $v_1 \leqslant v_2$, $v_2 \geqslant 176.07$. In sum,

$$102.14 \leqslant v_1 \leqslant 250, \quad 176.07 \leqslant v_2 \leqslant 250.$$

Based on the above ranges of reactor volumes and the product demands, lower and upper bounds on the number of batches for each product can be derived, as shown in Table 2.

The concave terms in the objective function are underestimated with 4-piece and 2-piece linear approximations. The branch and bound process

Table 1. Demand scenarios (unit: m^3/week)

Product	Scenario 1	Scenario 2
L1	2600	2600
L2	2300	2300
L3	450	1700
L4	1200	530
L5	560	530
L6	530	280
L7	530	250
L8	140	230
L9	110	160
L10	110	90
L11	10	70
L12	110	390
L13	90	250
L14	90	160
L15	90	100
L16	70	70
L17	50	50
L18	30	50
L19	10	50
L20	10	–
L21	10	–
L22	190	–
L23	180	–
L24	70	–
L25	70	–
L26	40	–
L27	40	–
L28	40	–
L29	30	–
L30	20	–
L31	20	–
L32	20	–
L33	10	–
L34	10	–
L35	10	–
L36	10	–
L37	10	–
Total	9870	9860

requires only one iteration to solve the problem to global optimality with a 0.05% gap (i.e., the gap between the upper bound and the lower bound at the root node of the branch and bound tree is within the stopping criterion and hence the search procedure can be terminated right after solving the root node). The MILP lower bounding problem consists of 69 binary variables, 124 continuous variables and 489 equations. The solution requires 1721 CPU s on an HP J-2240 workstation (note: the performance of this machine is close to that of a Pentium III Intel based PC). The optimal

Table 2. Ranges of number of batches for Scenario 2

Demand (m^3/week)	Products	Reactor 1 102.14–250 m^3	Reactor 2 176.07–250 m^3	Reactor 1 and 2
2600	1 (L1)	0–11	6–15	11–17[a]
2300	1 (L2)	0–11	5–14	10–16[a]
1700	1 (L3)	0–11	2–10	7–13[a]
530	2 (L4, L5)	0–6	0–4	3–6
390	1 (L12)	0–4	0–3	2–4
280	1 (L6)	0–3	0–2	2–3
250	2 (L7, L13)	0–3	0–2	1–3
230	1 (L8)	0–3	0–2	1–3
160	2 (L9, L14)	0–2	0–1	1–2
100	1 (L15)	1	X	1
90	1 (L10)	1	X	1
70	2 (L11, L16)	1	X	1
50	3 (L17–L19)	1	X	1

The third and fourth columns represent the number of batches for each product in Reactor 1 and Reactor 2, respectively; while the last column represents the total number of batches for each product in both reactors. When there are two numbers in the form of N^L–N^U, they represent the lower and upper bounds on the number of batches (e.g., for Product L1, the number of batches in Reactor 1 is in the range from 0 to 11); when there is only one number, it is the exact number of batches (e.g., for Product L17, there is exactly one batch in Reactor 1); X means no assignment is needed/possible (e.g., for Product L17, no batches are produced in Reactor 2).

[a] Derived based on the fact that at most 56 batches are available and the sum of the lower bounds is already 50.

solution is provided in Table 3 and the corresponding minimal total cost is $c^T = 31.809$.

4.2. A LARGE CASE STUDY: SCENARIO 1

Three reactors are introduced and the bounds of the reactor volumes can also be tightened. Because of the small demands of $10\,m^3$ (L11, L19–L21, L33–L37), the upper limit on surplus production, $S = 1$, and the lower limit of utilization rates, 0.4, one reactor has to be smaller than $10(1 + 1)/0.4 = 50\,m^3$. A total volume of $9870/28 = 352.5\,m^3$ is required, that is, $v_1 + v_2 + v_3 \geqslant 352.5$. It follows that $v_2 + v_3 \geqslant 302.5$, and hence $v_2 \geqslant 52.5$, $v_3 \geqslant 151.25$. In sum,

$$20 \leqslant v_1 \leqslant 50, \quad 52.5 \leqslant v_2 \leqslant 250, \quad 151.25 \leqslant v_3 \leqslant 250.$$

The range of the number of batches for each product, which is derived based on the ordering of product demands, is shown in Table 4.

The concave terms in the objective function are underestimated with 1-piece, 4-piece and 2-piece linear approximations. The branch and bound process requires again only one iteration to solve the problem to global

Table 3. Optimal slourion for Scenario 2

Product	Demand	Reactor 1: $v_1 = 132.5$ m^3			Reactor 2: $v_2 = 250$m^3		
	(m^3/week)	Production	Batches	Utilization rate	Production	Batches	Utilization rate
L1	2600	100	1	0.76	2500	10	1
L2	2300	1050	8	0.99	1250	5	1
L3	1700	0	0	–	1700	7	0.97
L4	530	530	4	1	0	0	–
L5	530	530	4	1	0	0	–
L6	280	53	1	0.40	250	1	1
L7	250	0	0	–	250	1	1
L8	230	0	0	–	230	1	0.92
L9	160	0	0	–	160	1	0.64
L10	90	90	1	0.68	0	0	-
L11	70	70	1	0.53	0	0	–
L12	390	390	3	0.98	0	0	–
L13	250	0	0	–	250	1	1
L14	160	0	0	–	160	1	0.64
L15	100	100	1	0.76	0	0	–
L16	70	70	1	0.53	0	0	–
L17	50	100	1	0.76	0	0	–
L18	50	100	1	0.76	0	0	–
L19	50	100	1	0.76	0	0	–
Total	9860	3283	28		6750	28	
				Total production: 10,033			

optimality with 0 gap. The MILP lower bounding problem consists of 124 binary variables, 263 continuous variables and 984 equations. The solution requires 741 CPU s on an HP J-2240 workstation. The optimal solution is provided in Table 5 and the corresponding minimal total cost is $c^{\mathrm{T}} = 37.176$. Note that due to the dramatic effect of the bounds imposed on the number of batches on the required computational time, we start with the reduced ranges in Table 4, which use very tight upper bounds. After the solution is obtained, the value of the number of batches for each product is examined. If any upper bounds are hit, they are increased and the problem is solved again, which leads to the same solution. This verifies that the tightened bounds on the number of batches do not cut off potentially better solutions and the global optimality of the obtained solution is guaranteed.

It should be pointed out that for each scenario, the reactor volumes in the solution given in this paper lead to the minimal total cost, however, in terms of the assignment of products to reactors and production amounts, the solution provided here may not be unique and can be one of the multiple solutions that exist.

Table 4. Ranges of number of batches for Scenario 1

Demand (m^3/week)	Products	Reactor 1 20–50 m^3	Reactor 2 52.5–250 m^3	Reactor 3 151.25–250 m^3	Reactor 1, 2 and 3
2600	1 (L1)	X	0–3	8–12	11–15
2300	1 (L2)	X	0–3	7–11	10–14
1200	1 (L4)	X	0–3	2–6	5–9
560	1 (L5)	0–2	0–4	0–4	3–4
530	2 (L6, L7)	0–2	0–4	0–4	3–4
450	1 (L3)	0–2	0–3	0–3	2–3
190	1 (L22)	0–2	0–2	0–2	1–2
180	1 (L23)	0–2	0–2	0–2	1–2
140	1 (L8)	0–2	0–2	0–1	1–2
110	3 (L9, L10, L12)	0–2	0–2	0–1	1–2
90	3 (L13–L15)	0–2	0–2	0–1	1–2
70	3 (L16, L24, L25)	0–2	0–1	0–1	1–2
50	1 (L17)	1–3	X	X	1–3
40	3 (L26–L28)	1–2	X	X	1–2
30	2 (L18, L29)	1–2	X	X	1–2
20	3 (L30–L32)	1	X	X	1
10	9 (L11, L19–L21, L33–L37)	1	X	X	1

The third, fourth, and fifth columns represent the number of batches for each product in Reactor 1, Reactor 2, and Reactor 3, respectively; while the last column represents the total number of batches for each product in all of the three reactors. When there are two numbers in the form of N^L–N^U, they represent the lower and upper bounds on the number of batches (e.g., for Product L1, the number of batches in Reactor 2 is in the range from 0 to 3); when there is only one number, it is the exact number of batches (e.g., for Product L11, there is exactly one batch in Reactor 1); X means no assignment is needed/possible (e.g., for Product L11, no batches are produced in Reactor 2).

4.3. COMPARISON WITH PREVIOUS APPROACHES

Kallrath (2003) introduced the problem investigated in this paper and presented results obtained with three different approaches. In the first approach, an MILP formulation was proposed to approximate the original MINLP model, which used equivalent linear constraints and an approximate piecewise objective function. This MILP formulation was essentially an approximation of the original problem. Due to this limitation, the solution was not accurate and no systematic method was proposed to evaluate or reduce the gap between the obtained approximate solution and the real optimal solution. Furthermore, it required a great amount of computational time to solve the MILP problem when the size of the model was large in the large case study involving a relatively large number of products.

In the other two approaches, Kallrath (2003) attempted to employ two commercial MINLP solvers connected to GAMS (Brooke et al., 1988) to solve the problem. The first solver, SBB, is a local MINLP solver and uses a branch and bound scheme. For the small case study, only suboptimal

Table 5. Optimal solution for Scenario 1

Product	Demand (m^3/week)	Reactor 1: $v_1 = 20$ m^3			Reactor 2: $v_2 = 100$ m^3			Reactor 3: $v_3 = 250$ m^3		
		Production	Batches	Utilization rate	Production	Batches	Utilization rate	Production	Batches	Utilization rate
L1	2600	0	0	–	100	1	1	2500	10	1
L2	2300	0	0	–	50	1	0.50	2250	9	1
L3	450	0	0	–	200	2	1	250	1	1
L4	1200	0	0	–	200	2	1	1000	4	1
L5	560	0	0	–	100	1	1	460	2	0.92
L6	530	0	0	–	300	3	1	230	1	0.92
L7	530	0	0	–	300	3	1	230	1	0.92
L8	140	0	0	–	140	2	0.70	0	0	–
L9	110	20	1	1	90	1	0.90	0	0	–
L10	110	20	1	1	90	1	0.90	0	0	–
L11	10	20	1	1	0	0	–	0	0	–
L12	110	20	1	1	90	1	0.90	0	0	–
L13	90	0	0	–	90	1	0.90	0	0	–
L14	90	0	0	–	90	1	0.90	0	0	–
L15	90	0	0	–	90	1	0.90	0	0	–
L16	70	0	0	–	70	1	0.70	0	0	–
L17	50	50	3	0.83	0	0	–	0	0	–
L18	30	30	2	0.75	0	0	–	0	0	–
L19	10	20	1	1	0	0	–	0	0	–
L20	10	20	1	1	0	0	–	0	0	–
L21	10	20	1	1	0	0	–	0	0	–
L22	190	0	0	–	190	2	0.95	0	0	–
L23	180	0	0	–	180	2	0.90	0	0	–
L24	70	0	0	–	70	1	0.70	0	0	–
L25	70	0	0	–	70	1	0.70	0	0	–
L26	40	40	2	1	0	0	–	0	0	–
L27	40	40	2	1	0	0	–	0	0	–
L28	40	40	2	1	0	0	–	0	0	–
L29	30	30	2	0.75	0	0	–	0	0	–
L30	20	20	1	1	0	0	–	0	0	–
L31	20	20	1	1	0	0	–	0	0	–
L32	20	20	1	1	0	0	–	0	0	–
L33	10	20	1	1	0	0	–	0	0	–
L34	10	20	1	1	0	0	–	0	0	–
L35	10	20	1	1	0	0	–	0	0	–
L36	10	20	1	1	0	0	–	0	0	–
L37	10	20	1	1	0	0	–	0	0	–
Total	9870	530	28		2510	28		6920	28	
					Total production: 9960					

solutions were generated after five hours of CPU time even when v_2 was fixed to the optimal value; for the large case study, only when very tight bounds on v_2 and v_3 were used, could the solver find a solution, which was still suboptimal. The second solver, BARON, is a global solver and applies a branch and reduce framework. For the small case study, it required 12 CPU hours to find the optimal solution and then to prove the global

Table 6. Comparison of proposed approach with previous approaches

Approach		Kallrath (2003)			This approach
		MILP approximation	SBB	BARON	
Small case study (Scenario 2)	Binary var.	230	3	3	69
	Integer var.	38	38	38	–
	Continuous var.	289	99	99	124
	Constraints	1162	66	66	489
	Obj. (cost)	31.66[a]	32.126[b]	31.809	31.809
	Gap (%)	n/a	>1	0	0.05
	CPU (s)	<60[c]	~18,000[c]	~43,200[c]	1721[d]
Large case study (Scenario 1)	Binary var.	447	3	3	124
	Integer var.	111	129	129	–
	Continuous var.	656	284	284	263
	Constraints	2155	197	197	984
	Obj. (cost)	37.176	38.506[e]	39.164[f]	37.176
	Gap (%)	n/a	2.5	12.8	0
	CPU (s)	~20,700[c]	~300[c]	~277,200[c]	741[d]

[a]Inaccurate, exact value is 31.809. [b]Obtained with v_2 fixed. [c]Pentium III 750 MHz. [d]HP J-2240 workstation. [e]Obtained with very tight bounds on v_2 and v_3. [f]Obtained with v_3 fixed.

optimality; for the large case study, even after v_3 was fixed to the optimal value, the solver could only find a suboptimal solution still far away from the optimal one after 77 h of CPU time. It is obvious that both solvers suffer from very weak initial lower bounds and extremely slow convergence between the upper bounds and the lower bounds.

Table 6 shows the comparison between the results from the aforementioned previous approaches and those from the approach we have proposed in this paper. It is demonstrated clearly that the improved model and the customized branch and bound approach is able to solve this nonconvex MINLP problem to global optimality rigorously and much more efficiently.

5. Conclusions

In this work, we address the global solution of a nonconvex MINLP problem arising from product portfolio optimization introduced by Kallrath (2003). The goal of the product portfolio analysis is to prove that complex portfolios lead to more costly scenarios caused by the requirement of more reactors. In order to do so we have formulated and solved optimization models to determine the optimal configurations of reactors with the minimal fixed and investment costs for two different scenarios of product demands. The model proposed by Kallrath (2003) is improved and the resulting mathematical formulation consists of a concave objective function and linear constraints with binary and continuous variables. A variety of techniques are developed to tighten the model and accelerate the convergence to the optimal solution. A customized branch and bound approach is proposed to solve the model to global optimality. Computational studies on the two scenarios are presented. In both cases, the global solutions are obtained and proved optimal very efficiently (i.e., essentially in one iteration), which demonstrate the effectiveness of the proposed approach.

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