Frontiers In Global Optimization, pp. 1-2
C. A. Floudas and P. M. Pardalos, Editors

Exact Computation of Global Minima of a Nonconvex Portfolio Optimization Problem

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Abstract

The goal of this project was to compute minimal cost solutions satisfying the demand of pre-given product portfolios and to investigate the dependence of the fix costs and investment costs on the product portfolio.

The most important parameters characterizing the production facilities are the number and the size of the reactors. The production is subject to shelf-life constraints, *i.e.*, products cannot be stored longer than one week.

Even if we analyze this problem under the simple assumption of constant batch sizes and limit ourself to only one time period covering one week, the computation of minimum cost scenarios requires that we determine global minima of a nonconvex MINLP problem. An objective function built up by the sum of concave functions and trilinear products terms involving the variables describing the number of batches, the utilization rates and the volume of the reactor are the nonlinear features in the model.

We have successfully applied four different solution techniques to solve this problem. (1) An exact transformation allows us to represent the nonlinear constraints by MILP constraints. Using piecewise linear approximations for the objective function the problem is solved with XPress-MP, a commercial MILP solver. (2) The local MINLP Branch-and-Bound solver SBB which is part of the modeling system GAMS. (3) The Branch&Reduce Optimization Navigator (BARON) also called from GAMS. (4) A taylorized Branch&Bound approach based on the construction of a lower bounding problem by underestimating the concave objective function with piecewise linear approximations described in a forecoming paper.

Our overall conclusion from a detailed analysis of specific portfolio cases is that the problem, for some cases, can be solved with nowadays standard solvers' capacities but it requires a lot of CPU time. Therefore, in order not to cover only special cases and also to cope with the scaling properties of this problem suffering from weak lower bounds, we recommend to use taylorized approaches in addition.

Keywords: Global Optimization, mixed integer programming, portfolio optimization, trilinear terms, concave objective functions, convex underestimators

1 Introduction

A business unit operating a few batch reactors wants to analyze the dependence of investment and fixed costs on given demand spectra. In this paper we analyze two different scenarios with fewer products than typically used in that business unit, *i.e.*, only 20 and 40 products: one including a new product with a capacity of 80.000 tons per year, the other one a "*lean* assortment" with fewer products. The current analysis should determine cost minimal solutions which also answer the following questions:

1. How many reactors are needed?
2. What capacity should those reactors have?
3. How many batches of each product are assigned to those reactors?

This analysis will help to define the optimal reactor configurations, and, in a second step, also to do a product portfolio analysis.

Section 2 contains a verbal description of the problem and some requirements regarding the optimization problem. *Section 3* contains the mixed integer nonlinear formulation of the problem. In *Section 4* we develop an alternative and equivalent MILP formulation. In *Section 5* we discuss two portfolio scenarios in great detail.

2 Problem Description

This section contains a verbal description of the problem and some requirements regarding the optimization problem.

2.1 Objectives and Expected Results

The objectives of this analysis is to support our client in proving that an extensive set of products in a portfolio does not necessarily maximize the profit. It may be much more efficient to design some *lean* product portfolios. To prove this conjecture we compute the global minimum of the investment and fixed operating costs for two different product scenarios. Besides the costs the following detailed results are expected:

- the number of reactors required and the number of batches per reactors
- 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

These questions can strictly only be answered using exact mathematical optimization techniques.

2.2 Constraints

The production network 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 shelf-life limits. Actually, the products can be stored for about one week; if they are appropriately cooled they can survive a few more days.

3. All products are produced in batches of 6 hours. The feasible volumes of the reactors are in the range between 20 and 250 m^3. The filling degree or utilization rate needs to be at least 40%.

4. For each reactor fixed costs and a nonlinear investment costs functions are known.

2.3 Costs

We consider only the following costs depending on reactors:

- *fixed costs;* regarding the fixed operating costs we should note that one person can control two reactors.

- *investments* costs; these are given for each reactor by a nonlinear concave function which relates the costs to the volume of the reactor.

Additional costs which one might think of, such as the costs of the production process, or costs related to the tanks have been neglected.

2.4 Some Remarks on the Accuracy of the Data

To prove our conjecture 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. Thus, the actual values of the cost data and also the demand data are of secondary importance.

2.5 Summary of the Relevant Input Data

The following input data determine the size of the problem:

- the potential number, N^{R}, of the reactors r, $2 \leq N^{\mathrm{R}} \leq 4$;

- the number, N^{P}, (20-40) of products p, $20 \leq N^{\mathrm{P}} \leq 40$;

- the maximal number, $N^{\mathrm{BR}} = 28$, of batches per reactor. This number results from the number of hours available per week (168) and the duration of the batches (6 hours).

If one considers all index combinations of reactors and products, it turns out the number of the nonlinear terms (products of three variables) are the critical quantity.

3 The Mathematical Optimization Model

This section describes the mathematical model.

3.1 Preliminaries

At first we give a brief summary of the indices, sets and variables.

3.1.1 Indices and Sets

In the model we use the following indices and dimensions:

$p \in \mathcal{P} := \{p_1, \ldots, p_{N^{\mathrm{P}}}\}$ for the products; $N^{\mathrm{P}} = 40$.
The products and their demand spectrum per week is pre-given.

$r \in \mathcal{R} := \{r_1, \ldots, r_{N^{\mathrm{R}}}\}$ for the reactors; $N^{\mathrm{R}} = 4$.

In the model we use the following variables (the units are shown in brackets):

3.1.2 Variables

We use the following variables:

v_r $[m^3]$ the volume of reactor r in m^3.
Those variables can vary between 20 and 250.

f_{rp} $[-]$ the filling degree or utilization rate of a reactor per batch.
Those variables can vary between 0.4 and 1.

p_p^{S} $[-]$ surplus production normalized to the demand.
Those variables can vary between 0 and 1.

t_r $[h]$ production time of reactors per week in hours.
It is useful to introduce this variable to implement the time-capacity constraint.

n_{rp}^{B} $[-]$ number of batches of reactor r and product p.
This is an integer variable taking values between 0 and 28 (in this specific case).

δ_r binary variable indicating that reactor r is active, *i.e.*, selected for production, and subject to investment cost.

c^{T} the total costs, presently only fixed operating costs and investment costs

c^{F} the fixed operating costs

c^{I} the investment costs

3.1.3 Input Data

The following input data need to be considered [units are shown in brackets]:

Costs:

C_r^{F} [kEuro/week] for reactor r.

C_r^{I} [$(k\mathrm{Euro})^2/\mathrm{m}^3$] investment cost or depreciation cost, resp., per m^3 for reactor r in each week.

Capacities and other production data:

C_r^{T} [hours] time capacity of reactor r; usually 168 hours, *i.e.*, the full week.

T_p^{P} [hours] time required to produce one batch of product p. This assumes that the production rates are constant and the same for all products and all reactors; 6 hours in the current case.

Demand:

Demand D_p [m^3] for product p per week considered. Values vary extremely between 2 and 15000.

Reactor data: The reactors are characterized by the minimal and maximal volumes and the limits on the utilization rate.

V_r^{L} [m^3] a lower limit on the reactor volume in case reactor r is active. This makes the volume variable, v_r, a semi-continuous variable.

V_r^{U} [m^3] an upper limit on the reactor volume in case reactor r is active.

F_r^{L} [-] the lower limit on the utilization or fill-up rates; this value, $F = F_r^{\mathrm{L}} = 0.4$, is the same for all reactors.

Production time:

C_r^{T} [hours] total time reactor r is available. Right now, we assume that all reactors have the same time availability; 168 hours in the analysis.

3.2 Model Formulation

3.2.1 Objective Function

It is the goal to minimize the total costs, *i.e.*, the sum, c^{T},

$$c^{\mathrm{T}} = c^{\mathrm{F}} + c^{\mathrm{I}} \tag{1}$$

of the fixed operating costs, c^{F}, given by the linear term

$$c^{\mathrm{F}} := \sum_{r \in \mathcal{R}} C_r^{\mathrm{F}} \delta_r \tag{2}$$

with $C_r^{\mathrm{F}} = 2.45k$Euro for all reactors, and the investment costs, c^{I}, depending nonlinearly on the volume of the reactors, *i.e.*,

$$c^{\mathrm{I}} := \sum_{r\in\mathcal{R}} \sqrt{C_r^{\mathrm{I}} v_r} \delta_r \quad . \tag{3}$$

The constant is given by $C_r^{\mathrm{I}} = 0.97(k\mathrm{Euro})^2/\mathrm{m}^3$ and is the same for all reactors. Note that the investment costs, c^{I}, are built up by a sum of concave functions.

3.2.2 Constraints

The total time a reactor is used cannot exceed the available time of that reactor, *i.e.*,

$$\sum_{p\in\mathcal{P}} T_p^{\mathrm{P}} n_{rp} \leq C_r^{\mathrm{T}} \delta_r \quad , \quad \forall\{r\} \quad . \tag{4}$$

Demand has to be satisfied

$$\sum_{r\in\mathcal{R}} p_{rp} = \sum_{r\in\mathcal{R}} n_{rp} f_{rp} v_r \geq D_p \quad , \quad \forall\{p\} \quad . \tag{5}$$

Note that only a fraction, f_{rp}, of the reactor volume, v_r, can be used, provided that we fulfill

$$F_r^{\mathrm{L}} \leq f_{rp} \leq 1 \quad , \quad \forall\{rp\} \quad . \tag{6}$$

For this analysis, $F = F_r^{\mathrm{L}} = 0.4$ is used. The difference, *i.e.*, the relative surplus production

$$p_p^{\mathrm{S}} := \left(\sum_{r\in\mathcal{R}} n_{rp} f_{rp} v_r - D_p \right) \Big/ D_p \quad , \quad \forall\{p\} \tag{7}$$

is bounded:

$$p_p^{\mathrm{S}} \leq S \quad , \quad \forall\{p\} \quad . \tag{8}$$

The right-hand-side reflects the fact that the product can be stored at most for one week. Therefore, 100% surplus production are allowed, *i.e.*, $S = 1$. We assume that the tank inventory has sufficient capacity.

Lower and upper bounds on reactor volume, if a reactor is chosen

$$V_r^{\mathrm{L}} \delta_r \leq v_r \leq V_r^{\mathrm{U}} \delta_r \quad , \quad \forall\{r\} \quad . \tag{9}$$

This can also be formulated using semi-continuous variables.

3.3 Improving the Model Formulation

The problem is, due to its symmetry, degenerated with respect to the reactor volume. This has a negative effect on the size of the B&B tree and the number of active nodes to be investigated. Therefore, we break the symmetry by requiring that the reactors are numbered and counted with increasing volume, *i.e.*, we require

$$v_1 \leq v_2 \leq \ldots \leq v_{N^{\mathrm{R}}} \quad . \tag{10}$$

Another degeneracy is due to the fact that there are products with the same demand. This symmetry can be broken by establishing some order in sets, $\mathcal{P}_D$, of products with the same demand D. We have applied this only to the case in which three reactors were required. If product p proceeds p' in such a set $\mathcal{P}_D$, *i.e.*, $D_p = D_{p'}$, we apply the inequality

$$\left(N^{\mathrm{BR}}\right)^2 n_{1p} + N^{\mathrm{BR}} n_{2p} + n_{3p} \leq \left(N^{\mathrm{BR}}\right)^2 n_{1p'} + N^{\mathrm{BR}} n_{2p'} + n_{3p'} \quad , \tag{11}$$

which establishes a tendency to assign the preceeding product to the larger reactors first.

The model can be formulated somewhat tighter by observing that the total reactor volume required needs to match the demand. Therefore, we apply the constraint

$$N^{\mathrm{BR}} \sum_{r \in \mathcal{R}} v_r \geq \sum_{p \in \mathcal{P}} D_p \quad , \tag{12}$$

where the factor $N^{\mathrm{BR}} = 28$ reflects that each reactor cannot have more than 28 batches per week. Further bounds on the volumes can be derived from the following considerations. Let $D_{\min}$ be the minimal demand for a product scenario. The volume of the smallest reactor is bounded by

$$v_1 \leq \frac{1+S}{F} D_{\min} \quad . \tag{13}$$

Similarly, we can exclude the assignment of certain products to certain reactors by setting

$$n_{rp} = 0 \quad , \quad \forall \left\{ rp \,\middle|\, V_r^{\min} > \frac{1+S}{F} D_p \right\} \quad . \tag{14}$$

These bounds are special cases of general upper bounds, N_{rp}^+, we can apply to n_{rp}. If $V_r^{\min}$ denotes the lower bound of the volume, v_1, reactor r can take, then N_{rp}^+ is given by

$$N_{rp}^+ = \left\lceil \frac{D_p}{V_r^{\min}} \right\rceil \quad ,$$

where the operator $\lceil \circ \rceil$ indicates the ceiling function, *i.e.*, the rounding-up to the next integer. For the large demand products these bounds are very weak when computed for the small volume reactor. Therefore, we used another approach to compute N_{rp}^+. We have solved a sequence of subproblems with the objective function $\max n_{rp}$ subject to all others constraints of the problem and bounds found previously. For many cases we have solved these problems to optimality within a few minutes. Then we defined

$$N_{rp}^+ = \min \left\{ N^{\mathrm{BR}}, \left\lceil \frac{D_p}{V_r^{\min}} \right\rceil, \max n_{rp} \right\} \quad . \tag{15}$$

The computation of lower bounds, N_{rp}^-, is more complicated because it is difficult to assign products to reactors in advance. Therefore, similarly to the computation of N_{rp}^+ we have computed N_{rp}^- by solving a sequence of subproblems with the objective function $\min n_{rp}$. These problems have been solved to optimality with a few minutes. Furthermore, we derived lower bounds for the sum $\sum_{r \in \mathcal{R}} n_{rp}$ by solving a sequence of subproblems

$$N_p^- := \min \sum_{r \in \mathcal{R}} n_{rp} \quad . \tag{16}$$

3.4 The Structure of the Optimization Problem

The problem described in Section 3.2 is a mixed integer nonlinear programming (MINLP) problem which simultaneously contains a design problem (determining the number and size of reactors) and an assignment problem (assigning products to reactors and production amounts). Due to the objective function and the trilinear terms it is nonconvex. Therefore, we need global optimization techniques to compute the optimum. Structurally, many combinations of the number of batches and the volumes might lead to similar or even the same objective function values. Thus, we may expect that in terms of the assignment of products to reactors and production amounts, the solution derived may not be unique and can be one of the multiple solutions that exist. Of course, due to the monotonously increasing investment costs there is a tendency to have the reactor values as small as possible.

Due to the concave investment costs one would expect a cost minimal solution with one small reactor (covering the small demands), a small-to-midsize reactor and a large reactor with a volume equal to 250 m^3. However, the surplus production restriction and the utilization or minimum filling rate might exclude this solution.

4 An Approximately Equivalent MILP Formulation

The nonlinear products $n_{rp} f_{rp} v_r$ are difficult terms in our optimization problem. However, they can be replaced by the auxiliary variables p_{rp}. In order to do so we introduce the binary representation of the integer number n_{rp}

$$\sum_{i=1}^{I_{rp}} 2^{i-1} \alpha_{rpi} = n_{rp} \quad , \quad \forall \{rp\} \quad , \tag{17}$$

where the variables $\alpha_{rpi} \in \{0,1\}$ are binary variables (binary representation) and I_{rp} is, as $N^{\mathrm{BR}} = 28$, less than 5. If reactor r is not active at all, then those variables α_{rpi} take the value 0. Therefore, we have

$$\alpha_{rpi} \le \delta_r \quad , \quad \forall \{rpi\} \quad . \tag{18}$$

Instead of (5) we therefore can write

$$p_{rp} = \sum_{i=1}^{I_{rp}} 2^{i-1} p_{rpi}^{T2} = \sum_{i=1}^{I_{rp}} 2^{i-1} \alpha_{rpi} f_{rp} v_r = n_{rp} f_{rp} v_r \quad , \quad \forall \{rp\} \tag{19}$$

and formally, but never explicitly in the model

$$p_{rpi}^{T2} := \alpha_{rpi} f_{rp} v_r \quad , \quad \forall \{rpi\} \quad .$$

The variables p_{rpi}^{T2} can be calculated by the following system of linear inequalities:

$$p_{rpi}^{T2} \le V_r^{\mathrm{U}} \alpha_{rpi} \quad , \quad \forall \{rpi\} \quad , \tag{20}$$

$$p_{rpi}^{T2} \le v_r \quad , \quad \forall \{rpi\} \quad , \tag{21}$$

$$p_{rpi}^{T2} \ge F_r^{\mathrm{L}} v_r - F_r^{\mathrm{L}} V_r^{\mathrm{U}} (1 - \alpha_{rpi}) \quad , \quad \forall \{rpi\} \quad . \tag{22}$$

This formulation requires some comments. For $f_{rp} = F_r^{\rm L} = 1$ the approach is obvious. The case $\alpha_{rpi} = 0$ leads to $p_{rpi}^{T2} = 0$, while $\alpha_{rpi} = 1$ generates the inequalities $p_{rpi}^{T2} \leq v_r$ and $p_{rpi}^{T2} \geq v_r$, *i.e.*, $p_{rpi}^{T2} = v_r$. Let us now focus on the variable f_{rp} describing the reactor utilization rate. In our model we just require that this utilization rate, f_{rp}, varies between $F_r^{\rm L}$ and 1. Note that this value is not explicitly required in the model. The inequalities (21) and (22) generate, for $\alpha_{rpi} = 1$, the chain of inequalities

$$F_r^{\rm L} \leq \frac{p_{rpi}^{T2}}{v_r} \leq 1 \quad ,$$

i.e., they are sufficient to ensure that the utilization and fill-up rates are within the required bounds.

To tighten the model, we apply additional upper bounds onto the contributing binary components

$$\alpha_{rpi} = 0 \quad , \quad \forall \left\{ nri \left| N_{rp}^{+} < 2^{i-1} \right. \right\} \tag{23}$$

$$\alpha_{rp1} = 1 \quad , \quad \forall \left\{ nr \left| N_{rp}^{-} = 1 \wedge N_{rp}^{+} = 1 \right. \right\} \tag{24}$$

and

$$p_{rpi}^{T2} \leq (1 + S) D_p \quad . \tag{25}$$

To stay within a MILP framework we use an SOS-2 type formulation [*cf.* Kallrath & Wilson (1997,[9])] of the objective function and replace (3) using $N^{\rm B} = 7$ breakpoints $V_{rb} = \{0$, 20, 30, 100, 110, 240, and $250\}$ by:

$$c^{\rm I} = \sum_{r \in \mathcal{R}} c_r^{\rm A} \tag{26}$$

$$c_r^{\rm A} = \sum_{b=1}^{N^{\rm B}} \sqrt{C_r^{\rm I} V_{rb}} \lambda_{rb} \quad ; \quad C_r^{\rm I} = 0.97 \quad , \quad \forall \{r\} \tag{27}$$

$$v_r = \sum_{b=1}^{N^{\rm B}} V_{rb} \lambda_{rb} \quad , \quad \forall \{r\} \quad , \tag{28}$$

and the convexity constraint

$$\sum_{b=1}^{N^{\rm B}} \lambda_{rb} = 1 \quad , \quad \forall \{r\} \quad , \tag{29}$$

where at most two variables of a set $\{\lambda_{r1}, \lambda_{r2}, \ldots, \lambda_{rb}, \ldots, \lambda_{rN_r^{\rm B}}\}$ are allowed to be different from zero; these two variables need to be adjacent with respect to their indices, *e.g.*, λ_{rb} and λ_{rb+1}. This SOS-2 set representation approximates the square root objective function by piecewise linear functions and allows us to compute the global optimum approximately.

Note that all relations required are in a model implementation are given with reference numbers while others, contained for mathematical reasoning only, are not numbered.

5 Discussing Specific Cases

We analyzed two different data sets which approximately lead to the same amount of total weekly demand of 9.870 and 9.860 m^3.

Prd	Scen1	Scen2	Prd	Scen1	Scen 2	Prd	Scen1	Scen2
L1	2.600	2.600	L14	90	160	L27	40	
L2	2.300	2.300	L15	90	100	L28	40	
L3	450	1.700	L16	70	70	L29	30	
L4	1.200	530	L17	50	50	L30	20	
L5	560	530	L18	30	50	L31	20	
L6	530	280	L19	10	50	L32	20	
L7	530	250	L20	10		L33	10	
L8	140	230	L21	10		L34	10	
L9	110	160	L22	190		L35	10	
L10	110	90	L23	180		L36	10	
L11	10	70	L24	70		L37	4	
L12	110	390	L25	70		L38	2	
L13	90	250	L26	40		L39	2	
						L40	2	

The names L1 to L40 refer to the products. The demand of all products corresponds to an annual capacity of 670.000 m^3, which, as the density is 1,3t/m^3, corresponds to 871.000 tons. Each batch takes 6 hours. The week has 168 hours, so the maximal number of batches on each reactor is $N^{BR} = 28$. Products can be stored at most for one week. Assuming that we have sufficient storage capacity to store one week's production, we can produce twice the amount specified by the demand, i.e., 100% surplus production. The volume of the reactors can vary between 20 and 250m^3. The required minimum volume filling rate is $F = 0.4$, *i.e.*, 40%.

If we inspect Scenario 1 with 40 products it becomes obvious that the small demands for the products L37 to L40 cannot be fulfilled on reactors with minimal volumes of 20m^3. The small demands can, in agreement with (13), only be satisfied on reactors which have a volume less than 10 m^3, *i.e.*, less than the minimum reactor volume possible. This accounts for 100% surplus production, and a 40% filling degree. But if the first reactor has a volume of only 10 m^3, then with the second one in addition there is only a total reactor volume available of 260 m^3. However, we need to satisfy 9870 m^3, *i.e.*, a total volume of at least $V_{\min} = 9870\text{m}^3/28 = 352.5$ m^3 is required. Thus, we need at least a third reactor.

In order to keep Scenario 1 and 2 consistent with respect to the total demand, we replace the demands L37 to L40 given above, by setting the demand for L37 equal to 10 m^3 and the demands for L38 to L40 to zero. Now, the largest reactor feasible for this demand with $F = 0.4$ and $S = 1$, is according to (13), 50 m^3. Thus, we add the bounds

$$20 \leq v_1 \leq 50 \quad . \tag{30}$$

As we need at least a total volume of $V_{\min}$ we can derive a lower bound on v_2 by inspecting

$$v_1 + v_2 + v_3 \geq V_{\min}$$

and

$$v_2 \geq V_{\min} - v_1 - v_3 \geq V_{\min} - \max(v_1) - \max(v_3) = 52.5 \quad . \tag{31}$$

If we combine $v_2+v_3 \geq V_{\min} - \max(v_1) = V_{23} = 302.5$ with the symmetry-breaking condition (10) we are able to derive a lower bound for v_3 by solving the following minimization problem

$$\begin{aligned} & \min v_3 \\ s.t. \quad v_2 + v_3 & \geq V_{23} \\ v_2 & \geq v_3 \quad . \end{aligned}$$

Using the substitution $v_2 = v_3 - 2\Delta$, $\Delta \geq 0$, this problem is equivalent to

$$\min v_3 \quad s.t. \quad 2v_3 \geq V_{23} + 2\Delta \quad ,$$

which obviously has the optimal solution $\Delta = 0$ and $v_3 \geq V_{23}/2$. Thus we get the additional bound

$$151.25 \leq v_3 \leq 250 \quad . \tag{32}$$

Based on (14), for Scenario 1 we have worked out additional bounds for the number of batches:

$$n_{rp} = 1 \quad ; \quad r \in \{1\} \quad , \quad p \in \{\mathrm{L11}, \mathrm{L19}-\mathrm{L21}, \mathrm{L33}-\mathrm{L36}\} \quad , \tag{33}$$

$$n_{rp} = 0 \quad ; \quad r \in \{2\} \quad , \quad p \in \{\mathrm{L11}, \mathrm{L19}-\mathrm{L21}, \mathrm{L33}-\mathrm{L36}\} \quad . \tag{34}$$

$$n_{rp} = 0 \quad ; \quad r \in \{3\} \quad , \quad p \in \{\mathrm{L11}, \mathrm{L17}-\mathrm{L21}, \mathrm{L26}-\mathrm{L36}\} \quad . \tag{35}$$

As Scenario 1 turns out to be numerically much more complicated we derive further bounds as described in Section 3.3 [if no bounds are specified for a product, no bounds have been derived or are not necessary due to (33) to (35)]:

p	L1	L2	L3	L4	L5 – L7	L8 – L37
N^-_{3p}	6	5	1	1	1	0
N^-_p	11	10	2	5	3	1

,

and

p	L17	L13 – L16, L24, L25	L22, L23
N^+_{1p}	3	2	4

,

p	L8 – L10, L12	L13 – L16	L17, L18, L26 – L32
N^+_{2p}	3	2	1

,

p	L1	L2	L3	L4	L5 – L7	L22, L23	L8-L10,L12-L16,L24,L25
N^+_{3p}	12	12	3	8	4	2	1

.

The computation were further supported by the upper bound, N^+_p, on the sum of batches for product p over all reactors. These data followed from inspecting the demand and known N^+_{rp} values:

p	L1	L2	L4	L5	L3, L17	L16, L24 – L29	L11, L19 – L21, L30 – L36
N^+_p	15	14	9	4	3	2	1

.

In the next three subsections we describe the results obtained using different approaches.

5.1 Solving an Approximately Equivalent MILP Problem

Numerically, Scenario 2 is easy [230 binary, 38 integer, in total 557 variables, 1162 constraints], and is solved in less than a minute of CPU time on a Pentium III processor running at 750 MHz. It turns out that in Scenario 2 two reactors are sufficient to satisfy the demand. The concave investment cost function let us expect that we have one reactor at maximum capacity, *i.e.*, 250 m^3, and the other one at some value just large enough to satisfy all demands. But this is only possible when both the surplus production, S, of 100% and the utilization rate, F, are within certain bounds.

It is interesting to see for which combinations of the values S and F we still get the optimal solution characterized by

$$c^{\mathrm{T}} = 31.66 \quad , \quad c^{\mathrm{F}} = 4.90 \quad , \quad c_1^{\mathrm{I}} = 11.21 \quad , \quad c_2^{\mathrm{I}} = 15.55 \quad . \tag{36}$$

The following table shows the input parameters, S and F, and the optimal reactor volumes, v_1 and v_2

scenario	F [%]	S [%]	v_1	v_2	Δ	δ
S2-37000	37	0	132.49	250	0.10	0.32%
S2-40100	40	100	132.49	250	0.10	0.32%
S2-60060	60	60	132.49	250	0.10	0.32%
S2-75100	75	100	132.49	250	0.10	0.32%

Δ is the integrality gap, and δ is the gap in percent, *i.e.*,

$$\delta := 100 \frac{\Delta}{c^{\mathrm{T}} - \Delta} \quad . \tag{37}$$

Due to the piecewise linear approximation of the objective function the value $c^{\mathrm{T}} = 31.66$ is somewhat inaccurate; the exact value should be $c^{\mathrm{T}} = 31.809$ but this is not really relevant here. The solution have been obtained within minutes. Note that optimal solutions without any surplus production exist. But, as is expected, in this case, the reactor utilization rate is small.

Due to increased number of products, Scenario 1 has 447 binary, 111 integer, in total 1214 variables and 2155 constraints and turns out to be very diffucult to solve. However, using the tightening bounds described in Section 3.3 and the commercial MILP solver `XPress-MP`[1] [see, for instance, Ashford & Daniel (1987,[4])] Release 13.26, we have found the optimal solution with three reactors

$$c^{\mathrm{T}} := 37.1758 \quad ; \quad v_1 = 20 \quad , \quad v_2 = 100 \quad , \quad v_3 = 250$$

after 2,352,017 nodes and have proven its optimality after $5^{\mathrm{h}}45^{\mathrm{m}}$ CPU time and evaluating 2,908,750 nodes. Note that the reactor volumes derived lead to the minimal total costs, however, in terms of the assignment of products to reactors and production amounts, the solution obtained here may not be unique and can be one of the multiple solutions that exist. It is interesting, but not quite unexpected that there is no surplus production; it keeps the total volume as small as possible and thus minimizes costs. The table gives the number of batches on each reactor and the associated utilization rate in percent. Example:

[1] `Xpress-MP` is a registrated trademark of Dash Optimization (http:/www.dashoptimization.com).

1) Product L17 is produced in 3 batches on reactor R1 (20 m^3); 1 at 100% and 2 at 75%. 2) Product L2 is produced in three batches on reactor R2 (100 m^3) and 8 batches on reactor R3 (250 m^3); all batches run at 100% leading to a total production of 2300 m^3.

Prd	Scen1	R1	R2	R3	Prd	Scen1	R1	R2	Prd	Scen1	R1
L1	2.600		1	10	L14	90		1/90	L27	40	2
L2	2.300		3	8	L15	90		1/90	L28	40	2
L3	450			2/90	L16	70		1/70	L29	30	2/75
L4	1.200		2	4	L17	50	1+2/75		L30	20	1
L5	560		1	2/92	L18	30	2/75		L31	20	1
L6	530		3	1/92	L19	10	1/50		L32	20	1
L7	530		3	1/92	L20	10	1/50		L33	10	1/50
L8	140		2/70		L21	10	1/50		L34	10	1/50
L9	110	1/50	1		L22	190		2/95	L35	10	1/50
L10	110	1/50	1		L23	180		2/90	L36	10	1/50
L11	10	1/50			L24	70		1/70	L37	10	1/50
L12	110	1/50	1		L25	70		1/70			
L13	90		1/90		L26	40	2				

Another optimal solution differs from this solution, for example, only by satisfying the demand for products L3 by R2(2)+R3(1), L9 by R1(1)+R2(1/90) and for L23 by R3(1/72). Note that in both solutions exactly 28 batches are assigned to each reactor.

Let us now compare these solutions with the results we obtain from genuine nonlinear solution techniques.

5.2 Computing Local and Global Solutions with SBB and BARON

The Branch&Bound algorithm `SBB` embedded in `GAMS`[2] [see, for instance, Broocke *et al.*, (1992, [5])] produces good solutions for the 20-product scenario [3 binary, 38 integer, in total 140 variables, 66 constraints, 116 nonlinear nonzeros], within minutes; an 8% gap is reached within 28 seconds. However, even when we fix $v_2 = 250$ and thus have only v_1 as a free design variable, after 5 hours CPU time we get an objective function value $c^{\mathrm{T}} := 32.1257$ corresponding to $v_1 = 140$ while the global optimum is $c^{\mathrm{T}} := 31.809$ and $v_2 = 132.5$ as has been shown in Section 5.1 and has also been proven in Lin *et al.* (2003, [10]).

The Branch&Reduce Optimization Navigator (`BARON`) exploiting global optimization techniques [see, for instance, Ghildyal and Sahinidis (2001,[8]) or Tawarmalani & Sahinidis (2002,[11])] shows better properties. Again, it is obvious for the scenarios tested that the solution process suffers from weak lower bounds which improve only very slowly. `BARON` produces the optimal solution $c^{\mathrm{T}} := 31.809$ of the 20-product scenario after 6 hours CPU time or 937,576 nodes, but needs about 12 CPU hours (1,799,845 nodes) on a Pentium III processor running at 750 MHz to prove global optimality as shown below:

[2]`GAMS` is a registrated trademark of GAMS Development Inc., Washington D.C. (http://www.gams.com).

```
==============================================================
 Itn. no. Open Nodes Total Time Lower Bound  Upper Bound
       1        1     000:00:02  0.304261D+02 0.360448D+02
       1        1     000:00:02  0.304261D+02 0.360448D+02
   50000      839     000:18:52  0.312646D+02 0.360448D+02
  100000      982     000:36:39  0.313380D+02 0.360448D+02
  150000      109     000:55:10  0.314518D+02 0.360448D+02
  200000      465     001:14:35  0.314725D+02 0.360448D+02
  250000     1454     001:34:14  0.314725D+02 0.360448D+02
* 279244      628     001:45:17  0.314884D+02 0.329303D+02
  300000      924     001:53:51  0.314884D+02 0.329303D+02
* 334972     1379     002:08:38  0.314884D+02 0.329303D+02
  350000      573     002:14:27  0.315018D+02 0.329303D+02
* 361747     1197     002:19:16  0.315018D+02 0.321257D+02
  400000     2036     002:34:46  0.315018D+02 0.321257D+02
  450000     1962     002:54:41  0.315133D+02 0.321257D+02
  500000     2039     003:14:39  0.315133D+02 0.321257D+02
  550000     1714     003:34:16  0.315230D+02 0.321257D+02
  600000     2035     003:54:38  0.315230D+02 0.321257D+02
* 636994     1347     004:09:27  0.315313D+02 0.321257D+02
  650000     2036     004:14:48  0.315313D+02 0.321257D+02
  900000     1238     005:55:09  0.315630D+02 0.321257D+02
* 937576      939     006:10:36  0.315652D+02 0.318093D+02
  950000      565     006:15:22  0.315671D+02 0.318093D+02
 1000000      976     006:36:07  0.315779D+02 0.318093D+02
 1500000     2040     010:04:02  0.317089D+02 0.318093D+02
 1750000     1428     011:53:08  0.317354D+02 0.318093D+02
 1799845        0     012:14:10  0.318093D+02 0.318093D+02
```

We have skipped those parts of the log-output which did not appear useful. Note how slowly the lower bounds increases.

However, we experienced even great difficulties when using SBB to solve Scenario 1 [3 binary, 129 integer, in total 416 variables, 197 constraints, 336 nonlinear nonzeros]. If we use the bounds

$$100 \le v_2 \le 250 \quad , \quad 234 \le v_3 \le 250 \tag{38}$$

and the initial value $v_2 = v_3 = 100$ we get the following solution $v_1 = 20$, $v_2 = 140$, $v_3 = 235$ and $c^{\mathrm{T}} := 38.506$. The gap is only 2.5%; the best lower bound is 37.11. If we used more generous bounds, we could not find a solution at all. We got the solution within a few minutes using a depth first strategy (`nodesel=1,varsel=1`).

```
MODEL STATISTICS
BLOCKS OF EQUATIONS         9     SINGLE EQUATIONS      197
BLOCKS OF VARIABLES        10     SINGLE VARIABLES      416
NON ZERO ELEMENTS         877     NON LINEAR N-Z        336
DERIVATIVE POOL             6     CONSTANT POOL           9
CODE LENGTH              3147     DISCRETE VARIABLES    132
```

However, it is remarkable that no integer feasible solution was obtained even when we fixed the reactor volumes to the optimal values 20, 100 and 250.

The global optimization solver BARON, connected to GAMS, produces within 8 minutes a solution with $c^{\mathrm{T}} := 38.550$ and $v_1 = 20$, $v_2 = 140$, $v_3 = 236.3636$ and $c^{\mathrm{T}} := 38.550$ which is in close agreement with the local solution obtained by SBB. When we fixed $v_3 = 250$ and used $V_2^{\min} = 52.5$ as the lower bound for v_2 following from the demand values, we got the following results with BARON:

```
==============================================================
 Itn. no. Open Nodes Total Time Lower Bound  Upper Bound
        1     1       000:00:07  0.344631D+02 0.454590D+02
        1     1       000:00:08  0.346403D+02 0.454590D+02
 *    158    52       000:00:36  0.347117D+02 0.453131D+02
 *    158    35       000:00:36  0.347117D+02 0.444092D+02
 *    208    34       000:00:47  0.347117D+02 0.442201D+02
 *    208    27       000:00:47  0.347117D+02 0.433827D+02
 *   2629    52       000:05:50  0.347117D+02 0.433612D+02
 *   5527    25       000:11:29  0.347117D+02 0.430249D+02
 *   5536    18       000:11:30  0.347117D+02 0.425847D+02
    50000    36       001:16:38  0.347117D+02 0.425847D+02
 *  81649    14       002:04:00  0.347117D+02 0.422452D+02
 *  82584    13       002:05:42  0.347117D+02 0.421711D+02
 *  82584    11       002:05:42  0.347117D+02 0.418241D+02
 *  82695    11       002:05:53  0.347117D+02 0.417155D+02
 *  82695     5       002:05:53  0.347117D+02 0.398818D+02
   100000    43       002:30:36  0.347117D+02 0.398818D+02
 * 114625    10       002:54:48  0.347117D+02 0.396732D+02
 * 126509     8       003:09:51  0.347117D+02 0.396288D+02
 * 126509     8       003:09:52  0.347117D+02 0.395887D+02
   150000    34       003:38:45  0.347117D+02 0.395887D+02
 * 150085     7       003:38:51  0.347117D+02 0.395460D+02
 * 150085     5       003:38:51  0.347117D+02 0.393893D+02
   200000    23       004:44:40  0.347117D+02 0.393893D+02
   250000    20       005:49:17  0.347117D+02 0.393893D+02
   300000    21       006:53:06  0.347117D+02 0.393893D+02
   350000    20       007:56:29  0.347117D+02 0.393893D+02
 * 386305     4       008:40:43  0.347117D+02 0.393387D+02
 * 386305     4       008:40:43  0.347117D+02 0.391638D+02
 * 386305     4       008:40:43  0.347117D+02 0.391638D+02
   400000    37       009:00:53  0.347117D+02 0.391638D+02
  3600000    28       077:31:20  0.347117D+02 0.391638D+02
==============================================================
```

The objective function value, $c^{\mathrm{T}} := 39.1638$, corresponds to a solution with $v_2 = 144.444$ which is still far away from the optimal solution $v_2 = 100$. Note that the lower and upper bound did not change between the nodes 400,000 and 3,600,000 at all. After 77 hours of

CPU time we stopped this numerical experiment.

With both, SBB and BARON, it is problematic that the initial lower bound is significantly smaller than the optimal solution and that the lower bounds does, if at all, increase only very slowly. At this level those solvers try to find integer feasible solution which do not exist. Therefore, it seems that those solvers follow too much a depth-first strategy.

5.3 Computing Global Solutions with Convex Underestimators

A taylorized Branch&Bound approach has been developed and applied by Lin *et al.* (2003, [10]) to solve the model to global optimality. The kernel of this approach is to construct a lower bounding problem by underestimating the concave objective function with piecewise linear approximations [Floudas (1995, [6])]. These ideas and techniques are similar to those in the algorithm and software package αBB and SMIN-αBB developed by Floudas and Adjiman [see, for instance, Adjiman *et al.* (1998a, [2]; 1998b, [3]; Floudas (2000, [7]); 2003, [1])]. For further details we refer the reader to the Lin *et al.* (2003, [10]) paper. Here we just summarize that the globally cost minimal solution $v_1 = 20$, $v_2 = 100$, $v_3 = 250$, and $c^{\mathrm{T}} = 37.1758$ has been obtained and proven to be optimal within 741 CPU seconds on an HP J-2240 workstation.

6 Conclusion

It was the goal to prove that complex portfolios lead to more costly scenarios caused by more reactors required. In order to do so we have computed the global minimum of the sum of investment and fixed costs with respect to the number and volume of the reactors. We used three modeling approaches to do so: solving the nonlinear nonconvex problem using GAMS with a variety of solvers (among them SBB and BARON), solving an equivalent linear representation of that model exploiting the special structure of the problem and using XPress-MP, and using a taylorized Branch&Bound approach based on the construction of a lower bounding problem by underestimating the concave objective function with piecewise linear approximations.

For the scenarios tested the solution process suffers from weak lower bounds which improve only very slowly. The equivalent linear representation approach provides the global solution for Scenario 2 within a few minutes while Scenario 2 requires almost 6 hours to prove optimality. The commercial solvers, SBB and BARON, produce solutions for the small, 20-product scenario; BARON needs about 12 CPU hours on a Pentium III processor running at 750 MHz to prove global optimality. For the 40-product scenario no solutions have been produced with either SBB and BARON, in 40 hours. Only the taylorized Branch&Bound coupled with convex underestimators shows reasonable scaling properties and generates the globally optimal solution of the 40-product scenario with reactors of size 20, 100 and 250 m^3 and the objective function value $c^{\mathrm{T}} = 37.1758$ in about 13 minutes.

Thus, our overall conclusion is that the problem, for some cases, can be solved with nowadays standard solvers' capacities but it requires a lot of CPU time. Therefore, in order not to cover only special cases and also to cope with the scaling properties, we recommend to use taylorized approaches in addition.

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