Optimal Storage Design for a Multi-Product Plant: A Non-Convex MINLP Formulation☆

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Abstract

We discuss a tank design problem for a multi product plant, in which the optimal cycle time and the optimal campaign size are unknown. A mixed-integer nonlinear programming (MINLP) formulation is presented, where non-convexities are due to the tank investment cost, storage cost, campaign setup cost and variable production rates. The objective of the optimization model is to minimize the sum of the production cost per ton per product produced. A continuous-time mathematical programming formulation is proposed and several extensions are discussed. The model is implemented in GAMS and computational results are reported for the two global MINLP solver BARON and LINDOGlobal as well as several nonlinear solvers available in GAMS.

Key words: Mixed-integer nonlinear programming, global optimization, storage design, cycle time, campaign length, lot sizing problem, continuous-time model

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1. Introduction

We consider a tank-sizing problem motivated by Kallrath (22) within a multi-product, multi-reactor, chemical reaction plant. There are different types of costs associate with the production process; *i.e.* variable production cost, variable inventory cost and campaign setup cost. The problem is to determine the optimal tank-size along with the optimal cycle time and campaigns, i.e., for each campaign, the campaign length and campaign production size has to be determined.

The problem contains in its kernel a lot-sizing problem, which frequently occurs in food or chemical process industry when multi-purpose plants are used, *i.e.* plants with machines or reactors that can be operated in different modes; for a review on simultaneous lot-sizing and planning problems see Sürie (36) or Drexl and Kimms (6). In each mode it is possible to produce several products according to free or fixed recipes (joint production) leading to a general mode-product relation: in a certain mode, several products are produced (with different maximal daily production capacity rates), and vice-versa, a product can be produced in different (but not all) modes. To switch between modes, a changeover is necessary, which results in a considerable loss of production time. Planning problems of this type, where the production of an item implies some discrete event are called lot sizing problems; for a survey on lot sizing problems see Kuik et al. (26). The lot-sizing problem is accompanied by a sequencing problem. On top of this problem we have to solve the design problem.

Our tank-sizing problem is subject to stochastic demand uncertainty which is treated in Section 6.4. You and Grossmann (2008a; 2008b; 2009) consider supply chain design with stochastic inventory management simultaneously and use a probabilistic model to also predict the safety stock levels by integrating stock-out probability with demand uncertainty. Unlike this approach, in Section 4.2 we use deterministic lower bounds on the tank level, which can represent some technical requirement (bottom level), or safety stock figured out by the marketing colleagues, mostly by exploiting experience and the ordering behavior of the customers. As the bottom levels are usually smaller than the safety stock level the lower bounds are rather the safety stock level. As these are pre-given by the marketing division we treat the lower bounds only as deterministic input data and as hard constraints. Of course, in reality the lower bounds would be violated from time to time, and then tanks are refilled. Being aware that the optimal tank size is the minimum tank level plus the size of the working inventory, our stochastic approach in Section 6.4 only affects the size of the working inventory.

The contribution of this paper is the development of a new mathematical model combining a non-convex nonlinear tank-design problem with a lot sizing problem. The solution of this optimization problem gives an optimal investment decision, balancing tank cost and setup-change costs. Lot sizing problems are usually solved in the context of linear problems. Following the arguments along Kallrath (23), we combine the nonlinear design problem and the more operative aspects such as campaign length and setup changes (the lot sizing part of the problem) simultaneously. The continuous-time model to formulate the problem, the specific properties of the model, model enhancements and the extensions to more general cases are the main contributions of the paper.

The problem is described in Section 2. In particular, the goal of the optimization model and its constraints are discussed. Discrete and continuous-time optimization models are compared in Section 3 along with a justification why a continuous-time mathematical programming formulation is proposed in Section 4. Section 5 considers the properties of the mathematical programming formulation and gives an alternative formulation with convex mixed-integer constraints. Some generalizations of the model are discussed in Section 6 including the extension to cope with uncertain demand. Computational tests are performed in Section 7. We conclude with Section 8. All indices, sets, variables and input data are summarized in the appendix.

2. Problem Description

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

Given is a chemical plant with one reactor and P products $p \in \mathcal{P} := \{1, 2, \ldots, P\}$; we generalize this to R reactors in Section 6.2. We have to determine a production schedule satisfying the demands for each product and minimum as well as maximum storage capacities for each product. Furthermore, we want to determine the optimal size of the tank for each product.

2.1. Goals and Expected Results

The goal of this analysis is to support our client in the analysis of designing his tank storage equipment. Besides the costs, see Section 2.3, the following detailed results are expected:

- the cycle time T [days],
- the products tank sizes s_p^M [tons],
- the production of the campaigns p_{pn}^C [tons],
- the length of the campaigns t_n [days], and
- the number of mode-changes M [-].

These questions can strictly only be answered using exact mathematical optimization techniques. Note that there might exist several incommensurable cycle times.

The objective function requires further discussions. It is obvious that the total cost increase with the cycle time T monotonously. Hence, it is not meaningful to minimize the *total* cost. Instead, the most reasonable scenario seems to be to minimize the *costs per ton*, *i.e.*, we divide the total costs by the total production amount produced in a cycle, see Section 4.1. Some care is required to scale the tank investment costs appropriately.

2.2. Constraints

The production network is subject to the following constraints:

- The campaigns are subject to minimum and maximum production bounds, C_p^- [tons] and C_p^+ [tons].
- If a reactor is switched to a certain mode, it does so with a continuous production rate, p_{pn}^{R}, which has the physical units [tons/day]. The rate, p_p^{R}, may vary between the bounds $P_p^{\mathrm{R}-}$ [tons/day] and $P_p^{\mathrm{R}+}$ [tons/day].
- The reactors charge to a tank; this process happens in zero time.
- The size[1] of the tanks are subject to a minimum and maximum amount, S_p^- [tons] and S_p^+ [tons].

[1] For notational convenience, the tank sizes are measured in tons rather than in m^3. We can also justify the usage of m^3 as the chemical products stored have all density of approximately 1 $\mathrm{g/cm}^3$.

The demand for each product has to be satisfied. As we assume a period production schedule repeating itself after time horizon T, we require a non changing demand for each possible planning horizon T. Hence, we have to assume that the demand for each product p is constant throughout time. Given the annual demand, D_p [tons/year], of each product p, the continuous delivery rates L_p [tons/day] are then derived as

$$L_p := \frac{D_p}{365[\text{days/year}]} \quad . \tag{1}$$

With this assumption, the demand data are rough estimates for the 'real' demand.

2.3. Costs

We consider the following costs, given in [$]:

- *Variable production cost* c^{P}: The variable cost associated with the production of all products during the planning horizon T.
- *Setup cost* c^{C}: The sum of the production setup costs over all campaigns. No sequence-dependence is considered in the initial model.
- *Variable storage cost* c^{S}: The product dependent cost associated with the tank inventory over the planning horizon T. They reflect the capital binding costs as well as the operating costs.
- Tank *investments costs* c^{I}: For each tank, a (nonlinear) function relates the investment cost to the size of the tanks. The most important structural feature is that the *tank investment cost* – versus – *tank size function* is concave, see Section 4.1.
  We model the two cases when the tank can either be ordered at a design size (Section 4.1) or has to be purchased from a set of given tanks (Section 6.3).

Additional costs which one might think of, such as the fixed production costs, have been neglected.

3. Discrete versus Continuous-Time Models

In this section, we discuss the advantages and disadvantages of discrete versus continuous-time model formulations. This leads to a justification why we use a continuous-time model for our problem.

Discrete-time formulations are usually used in planning problems, less frequently, in scheduling problems; *cf.* Kallrath (21) or the literature review by Sürie (36). Continuous-time formulations have been successfully applied in the chemical industry [*cf.* Ierapetriou and Floudas (1998a; 1998b), Ierapetriou et al. (15), Lin and Floudas (27), Lin et al. (28), Jia and Ierapetritou (20), Janak et al. (19), Maravelias and Grossmann (31), Floudas and Lin (10), Castro and Grossmann (2005; 2006), Castro et al. (5), Shaik et al. (35), Shaik and Floudas (33), Janak and Floudas (16) and Floudas (8) for up-to-date reviews on scheduling in the process industry using mixed-integer linear programming and, in particular, continuous-time formulations, and to Janak et al. (2006a; 2006b) and Shaik et al. (34) for a large-scale industrial case study]. A comparison of discrete versus continuous-time formulations has been provided by Floudas and Lin (9).

To formulate a discrete-time model for our problem, we would have to select an appropriate *discretization* of the planning horizon. However, this might not be straight forward, especially when the length of the planning horizon is not known or very large. We could either select a sufficiently large horizon which fully includes the optimal cycle time, or we would discretize the interval [0,1] and multiply it with the unknown cycle time. For our investment problem, we have take into account the whole life-cycle of the tanks build. This may lead to a computationally intractable discrete-time model.

Continuous-time formulations appear natural in the context of unknown campaign length and unknown optimal cycle time. They also allow us, in case of unknown product demand for the discrete-time steps, to work with continuous delivery rates instead of a discrete-time estimation of the demand. The only disadvantage of continuous-time formulations we see is that it is a challenging task to compute an optimal number of event points needed in a cycle. Taking into account these arguments, we propose to use a continuous-time formulation.

4. Mathematical Model Formulation

This section describes a continuous-time mathematical programming formulation solving the described problem. The formulation is a non-convex mixed-integer nonlinear programming (MINLP) problem which will be extended in several ways in Section 6. All indices, sets, variables and data are summarized in the appendix.

Ideally, we want to have a model with unknown cycle time and unknown number of event points. As the event points have the status of indices in our *monolithic* model, we have to fix their number. Alternatively, in *polylithic*[2] approaches we could increase the number of event points dynamically.

To start with, let us consider and solve the model for a fixed number, N, of event points or campaigns $n \in \mathcal{N} := \{1, 2, \ldots, N\}$. Hence, we allow N discrete decisions over time for the production, namely which campaign to select at event point n. However, the length of each campaign is not fixed and will be determined by the model. The number of event points N implies then the maximal number of mode-changes M. If $N < N_*$, where N_* is the unknown optimal number of event points, and all event points are active, *i.e.*, they are associated to a campaign of non-zero duration, we might have missed the optimal solution. As we are not able to determine *a priori* an optimal number of event points, a steady increase of N yielding the same objective function value gives a good (heuristic) indicator that a global optimum has been reached (with respect to N). The numerical experiments in Section 7 will tell us that the computational effort with increasing N is mostly spend for proving optimality rather than computing an optimal solution.

In order to model the assignment decision of product $p \in \mathcal{P}$ for event point $n \in \mathcal{N}$, we introduce the binary variables

$$\omega_{pn} = \begin{cases} 1, & \text{if product } p \text{ is produced during time period } n \\ 0, & \text{otherwise} \end{cases} .$$

This allows us to model the production amount of product p during period n via the non-negative variable p^{C}_{pn}. Furthermore, we have to decide how long each campaign lasts. Therefore, introducing N non-negative continuous variables t_n defined through the sum of the non-negative production period, d_n, and the non-negative setup time t^{SC}_n. The sum over all event points of the

[2]The term "*polylithic*" has been coined by Kallrath (23).

production periods defines the planning horizon, T, which enters the model as a non-negative continuous variable.

Non-negative continuous variables s_{pn} keep track of the tank stock for period n and product p. We Define the tank size for each of the tanks as additional non-negative continuous variables s_p^M for each tank corresponding to product p.

4.1. Objective Function

The total costs c^{T} are given by the sum of the campaign setup costs c^{C}, the variable production cost c^{P}, the tank investment costs c^{I} and the tank storage costs c^{S}:

$$c^{\mathrm{T}} = c^{\mathrm{C}} + c^{\mathrm{P}} + c^{\mathrm{I}} + c^{\mathrm{S}} \quad . \tag{2}$$

The *campaign setup cost* c^{C} are given by

$$c^{\mathrm{C}} = \sum_{p\in\mathcal{P}} \sum_{n\in\mathcal{N}} C_p^{\mathrm{C}} \omega_{pn} \quad , \tag{3}$$

with the given fixed setup cost C_p^{C} [$] for each product p.

The *variable production cost* c^{P} are given by

$$c^{\mathrm{P}} = \sum_{p\in\mathcal{P}} C_p^{\mathrm{P}} L_p T \quad , \tag{4}$$

with C_p^{P} [$/ton] being the variable production cost for product p.

The *tank investment costs* are given for a time horizon of H years; a typical value for H is 5 years. These costs are concave and have the shape shown in Figure 1.

Normalized to the cycle time T, they are given by

$$c^{\mathrm{I}} = \frac{T}{365H[\text{days/year}]} \sum_{p\in\mathcal{P}} f(s_p^M, p) \quad , \tag{5}$$

where $f(x,p)$ is given, for instance, by

$$f(x) = A + \sqrt{Bx} \quad . \tag{6}$$

In the current case $f(x,p)$ reads

$$f(x,p) = C_p^{\mathrm{F}} + C_p^0 x^{0.5} \quad ; \quad C_p^{\mathrm{F}} := 165187 \quad , \quad C_p^0 := 0.21 \cdot 2274 \quad . \tag{7}$$

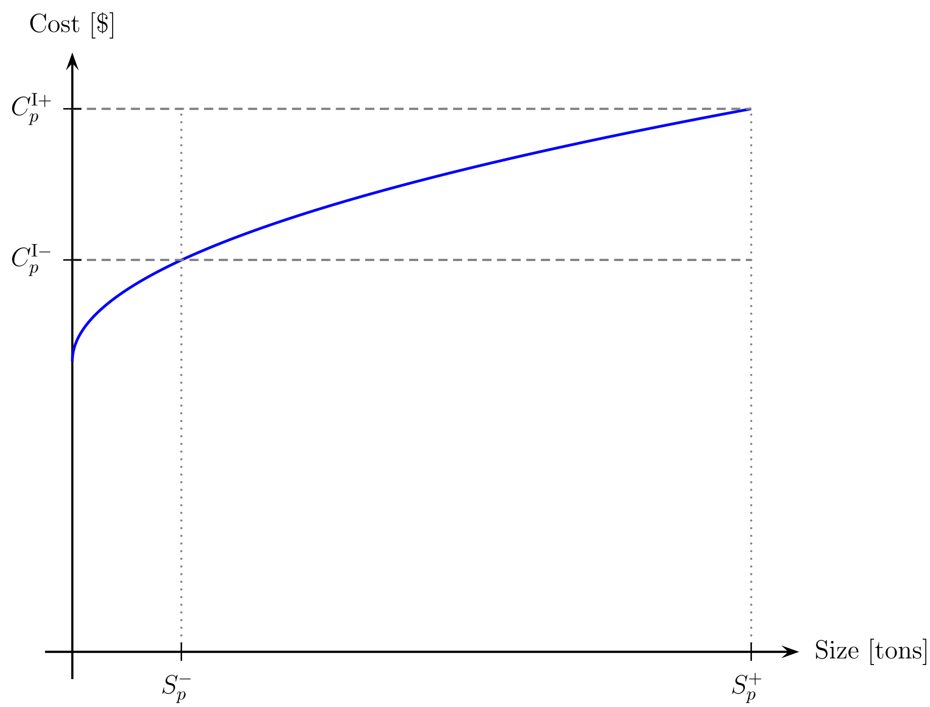


Figure 1: Tank investment cost with lower bound $C_p^{\mathrm{I}-}$ and upper bound $C_p^{\mathrm{I}+}$ over a 5 year horizon given as a concave function

Note that x in (7) has to be specified in tons to be consistent with the coefficient C_p^0.

An alternative formulation of the tank investment cost for discrete tank sizes – rather than a continuum – is given in Section 6.3.

The *variable tank costs* c^{S} depend more on the model formulation and are discussed at the end of Section 4.2.

As the total production, p^{T}, depends on the cycle length T, it is not meaningful to minimize the total cost. Instead, we minimize the cost per ton[3]

$$c^{\mathrm{PT}} := \frac{c^{\mathrm{T}}}{p^{\mathrm{T}}} = \frac{1}{365HL} \sum_{p \in \mathcal{P}} f(s_p^M, p) + \sum_{p \in \mathcal{P}} C_p^{\mathrm{P}} \frac{L_p}{L} + \frac{c^{\mathrm{C}} + c^{\mathrm{S}}}{LT} \quad , \tag{8}$$

or equivalently

$$c^{\mathrm{PT}} = \frac{1}{365HL} \sum_{p \in \mathcal{P}} \left(C_p^{\mathrm{F}} + C_p^0 \sqrt{s_p^M} \right) + \sum_{p \in \mathcal{P}} C_p^{\mathrm{P}} \frac{L_p}{L} + \frac{c^{\mathrm{C}} + c^{\mathrm{S}}}{LT} \tag{9}$$

with the total demand per day

$$L := \sum_{p \in \mathcal{P}} L_p \quad . \tag{10}$$

As the demand per day L [tons/day] is given, C_p^{F} of the tank investment cost reduce to fixed cost. Also, the variable production cost are fixed for each ton produced, which is clear as we assume that the variable production cost for each product are constant throughout time. Hence, those terms can be excluded from the model.

In order to avoid the division of variables, we minimize c^{PT} determined through relation

$$\begin{aligned} c^{\mathrm{PT}} TL &= c^{\mathrm{T}} = c^{\mathrm{C}} + c^{\mathrm{S}} + \frac{T}{365H[\text{days/year}]} \sum_{p \in \mathcal{P}} C_p^0 \sqrt{s_p^M} + \\ &\qquad + \sum_{p \in \mathcal{P}} \left(\frac{T}{365HL} C_p^{\mathrm{F}} + C_p^{\mathrm{P}} \frac{L_p T}{L} \right) \quad . \end{aligned} \tag{11}$$

[3] Note that the total costs depend on the planning horizon as the demand per day is fixed (and constant). However, the planning horizon is the unknown cycle time which enters as variable T in the model. As a consequence, minimizing the total cost leads indirectly to a minimization of T, eventually to zero. A more meaningful objective is to minimize the cost per ton produced (leading to a theoretical infinite planning horizon).

Recognize that the last sum in equation (11) is a constant for variable c^{PT} when the demand is given.

4.2. Constraints

The binary variable ω_{pn}, indicating whether product p is produced in campaign n, are subject to the constraint

$$\sum_{p \in \mathcal{P}} \omega_{pn} \leq 1 \quad , \qquad \forall n \in \mathcal{N} \quad , \tag{12}$$

i.e., at most one product can be produced in each campaign. The '$\leq$' is important to show that the optimal objective function values are monotonously decreasing with respect to the number of event points, see Section 5.1.

The sum of the lengths t_n of all periods n has to equal the cycle time T, *i.e.*,

$$\sum_{n \in \mathcal{N}} t_n = T \quad . \tag{13}$$

Given the setup-times through

$$t_n^{\mathrm{SC}} = \sum_{p \in \mathcal{P}} T_p^{\mathrm{S}} \omega_{pn} \quad , \qquad \forall n \in \mathcal{N} \quad , \tag{14}$$

the length of each campaign and possible setup-times is constrained by

$$t_n = d_n + t_n^{\mathrm{SC}}, \qquad \forall n \in \mathcal{N} \quad . \tag{15}$$

There might exist semi-continuous lower bounds D_{pn}^{-} on the lengths of the campaigns d_n depending on which product to be produced, *i.e.*,

$$d_n \geq \sum_{p \in \mathcal{P}} D_{pn}^{-} \omega_{pn} \quad , \qquad \forall n \in \mathcal{N} \quad . \tag{16}$$

Similarly, one could consider upper bounds D_{pn}^{+} by

$$d_n \leq \sum_{p \in \mathcal{P}} D_{pn}^{+} \omega_{pn} \quad , \qquad \forall n \in \mathcal{N} \quad . \tag{17}$$

The bounds D_{pn}^{-} and D_{pn}^{+} depend on the production rates, loss rates, lower and upper bounds of the storage tanks as well as minimum and maximum length of the campaigns. Notice that equations (17) imply that if thee is no production at all for an event point, then the duration of this event point is 0. One way to allow 'empty' campaign is to add an additional dummy product with zero demand.

With the production length d_n of period n at hand, the production during period n can then be described by

$$p^{\mathrm{C}}_{pn} = p^{\mathrm{R}}_{pn} d_n \omega_{pn} \quad , \qquad \forall p \in \mathcal{P}, \quad \forall n \in \mathcal{N} \quad , \tag{18}$$

where p^{C}_{pn} is the amount of product p produced in campaign n. Recognize that constraint (18) is trilinear; a mixed-integer linear programming formulation for this constraint is given in Section 5.4. The production rate p^{R}_{pn} specified in [tons/day] may be bounded by

$$P^{\mathrm{R}-}_{p} \le p^{\mathrm{R}}_{pn} \le P^{\mathrm{R}+}_{p} \quad , \qquad \forall p \in \mathcal{P}, \quad \forall n \in \mathcal{N} \quad . \tag{19}$$

At least the upper bound needs to be specified. Note that p^{R}_{pn} may vary from campaign to campaign.

There might exist a semi-continuous lower bound

$$p^{\mathrm{C}}_{pn} \ge C^{-}_{p} \omega_{pn} \quad , \qquad \forall p \in \mathcal{P}, \quad \forall n \in \mathcal{N} \tag{20}$$

and a semi-continuous upper bound

$$p^{\mathrm{C}}_{pn} \le C^{+}_{p} \omega_{pn} \quad , \qquad \forall p \in \mathcal{P}, \quad \forall n \in \mathcal{N} \tag{21}$$

on the production amount p^{C}_{pn}. Those bounds are usually given indirectly by the tank capacities and the minimum campaign duration as well as minimum batch sizes.

The model implements periodic constraints on the inventory, *i.e.*,

$$s_{pN+1} = s_{p1} \quad , \qquad \forall p \in \mathcal{P} \quad , \tag{22}$$

where the initial tank filling s_{p1} has to be specified. We will discuss the meaning of these constraints and the initial conditions in Section 4.4.

The amount of product stored in the tanks has to fulfill the bounds

$$S^{-}_{p} \le s_{pn} \le s^{M}_{p} \le S^{+}_{p} \quad , \qquad \forall p \in \mathcal{P}, \quad \forall n \in \mathcal{N} \quad . \tag{23}$$

The lower bounds on the inventory level S^{-}_{p} can represent some technical requirement (bottom level), or safety stock. As the bottom levels are usually smaller than the safety stock level we only consider the safety stock level.

The safety stock levels are figured out by the marketing colleagues, mostly by exploiting experience and the ordering behavior of the customers. In our analysis they are only treated as input data. The upper bound, S_p^+, is the maximal size of the tank available for each product.

The material balance constraints for each product p and period n are

$$s_{pn+1} = s_{pn} + p_{pn}^{\mathrm{C}} - L_p t_n \quad , \qquad \forall p \in \mathcal{P}, \quad n \in \mathcal{N} \quad , \tag{24}$$

stating that the storage amount of product p at the end of period n is given by the storage amount of product p at the beginning of period n minus the demand for product p during this period plus the produced amount of product p, if product p is produced in period n.

Finally, we are able to derive the *variable inventory costs* as

$$\begin{aligned} c^S &= \sum_{p\in\mathcal{P}}\sum_{n\in\mathcal{N}} \left[C_p^S \int_0^{t_n} (s_{pn} - L_p^{\mathrm{R}} t)\mathrm{d}t + C_p^S \int_0^{d_n} p_{pn}^{\mathrm{R}} t\omega_{pn} d\mathrm{t} \right] \qquad (25) \\ &= \sum_{p\in\mathcal{P}}\sum_{n\in\mathcal{N}} \left[C_p^S \int_0^{d_n+t_n^{\mathrm{SC}}} (s_{pn} - L_p^{\mathrm{R}} t)\mathrm{d}t + C_p^S \int_0^{d_n} p_{pn}^{\mathrm{R}} t\omega_{pn} dt \right] \\ &= \sum_{p\in\mathcal{P}}\sum_{n\in\mathcal{N}} C_p^S s_{pn} \left(d_n + t_n^{\mathrm{SC}}\right) + \\ &\qquad + \frac{1}{2} C_p^S \sum_{p\in\mathcal{P}}\sum_{n\in\mathcal{N}} \left[-L_p^{\mathrm{R}} \left(d_n + t_n^{\mathrm{SC}}\right)^2 + p_{pn}^{\mathrm{R}} \omega_{pn} d_n^2 \right] \\ &= C_p^S \sum_{p\in\mathcal{P}}\sum_{n\in\mathcal{N}} \left[s_{pn} d_n - L_p^{\mathrm{R}} t_n^{\mathrm{SC}} d_n + s_{pn} t_n^{\mathrm{SC}} - \right. \\ &\qquad \left. - \frac{1}{2} L_p^{\mathrm{R}} t_n^{\mathrm{SC}} t_n^{\mathrm{SC}} + \frac{1}{2} p_{pn}^{\mathrm{C}} d_n - \frac{1}{2} L_p^{\mathrm{R}} d_n^2 \right] \quad . \qquad (26) \end{aligned}$$

The first integrand of constraint (25) calculates the tank level s_{pn+1} of product p at the end of period n, if product p is not produced during that period. Recognize that we assume the demand to be continuous and constant throughout time, see Section 2.2. The second integrand corresponds to the production of product p during period n. Recognize that equation (26) contains $3\,(P \cdot N + N)$ bilinear terms.

The tank and production level throughout campaign n for a product p are drawn in Figure 2. The figure shows that the tank storage level decreases at a constant rate during the campaign setup time $T_p^{\mathrm{S}} = t_n^{\mathrm{SC}}$ and that there is no production during that time.

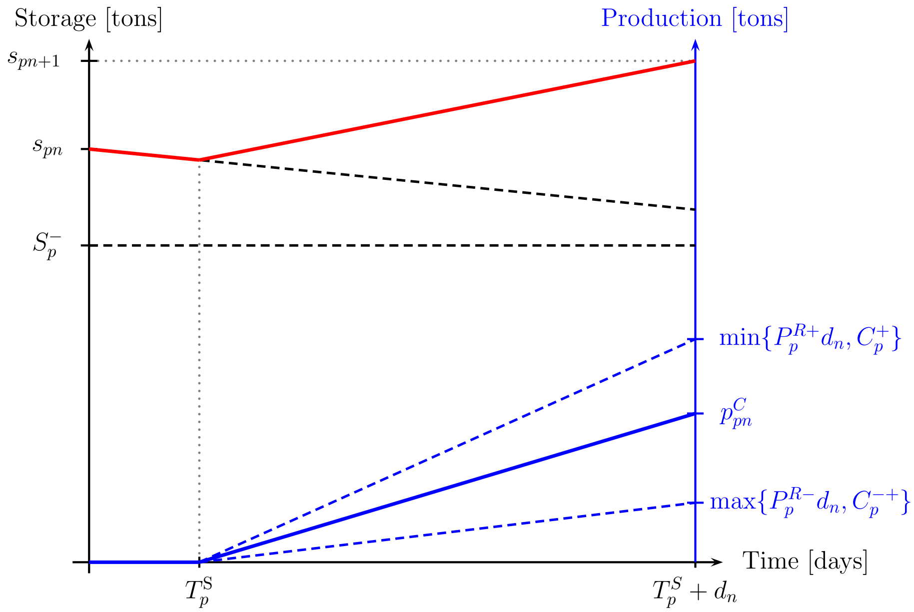


Figure 2: Tank storage level and production during period n for product p

The constant demand throughout time is an artificial assumption, necessary for our model to be consistent; see Section 2.2. Hence, the variable inventory cost given in equation (25) are only an approximation of the 'real' inventory cost. In order to reduce unnecessary complications at this point and to make the model simpler at the same time, we assume that the outflow and inflow of stock is constant throughout the *whole* period n. In this case, the variable inventory cost are just given by

$$c^{\mathrm{S}} = \sum_{p \in \mathcal{P}} C_p^{\mathrm{S}} \sum_{n \in \mathcal{N}} \frac{1}{2} \left[s_{pn+1} + s_{pn} \right] t_n \quad . \tag{27}$$

Note that s_{pn+1} means $s_{p,n+1}$, but we want to avoid the extra comma separating the first and second index. We do not expect confusion because the indices p and n are never multiplied with each other.

In order to reduce the number of nonlinear terms, we introduce the auxiliary variables

$$s_{pn}^{\mathrm{H}} := \frac{1}{2}(s_{pn+1} + s_{pn}) \quad , \qquad \forall p \in \mathcal{P}, \quad \forall n \in \mathcal{N} \quad . \tag{28}$$

Using these variables the variable inventory costs take the form

$$c^{\mathrm{S}} = \sum_{p\in\mathcal{P}} C_p^{\mathrm{S}} \sum_{n\in\mathcal{N}} s_{pn}^{\mathrm{H}} t_n \quad . \tag{29}$$

Notice that constraint (29) involves 'just' $P \cdot N$ bilinear terms.

The presented optimization problem is schematically shown in Figure 3. One can see the coupling of the lot-sizing problem with the tank design problem via the production variables p_{pn}^{C} and the demand delivery $L_p t_n$.

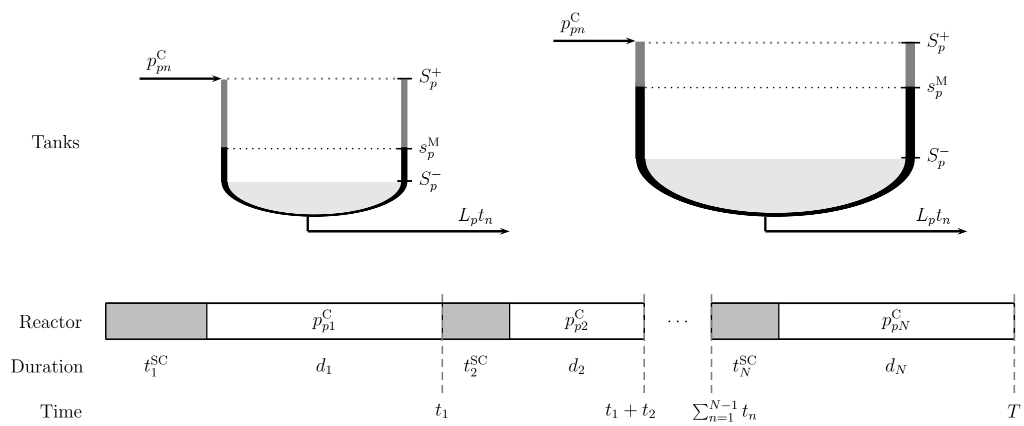


Figure 3: Schematic model of the optimization problem.

4.3. Demand Constraints

The production for all products p over the time horizon T has to satisfy the demand, *i.e.*,

$$\sum_{n\in\mathcal{N}} p_{pn}^{\mathrm{C}} = L_p T \quad , \qquad \forall p \in \mathcal{P} \quad . \tag{30}$$

Interestingly, this constraint is implied by the periodicity requirement for the tank inventory, constraints (22), and the material balance constraints (24) and, hence, redundant.

4.4. Initial Tank Levels

Consider again the periodicity constraints (22) on the initial and final inventory level. The reason for this constraint is to avoid disturbances at the end of the planning horizon. Having no constraint on the inventory level for the last period will certainly lead to the effect that any optimal solution empties the tanks as much as possible. This is very similar to mid-term operation planning for hydro-plants, where those effects are avoided by choosing a larger planning horizon (38).

Choosing the periodicity constraints (22) does solve the problem of avoiding those end-of-the planning horizon effects, however, there is a major drawback. What should we do with the initial inventory s_{p_1} for all products $p \in \mathcal{P}$?

One possibility is to fix some / all initial inventory to specific values; *i.e.*, the known values at the beginning of the design problem. However, in this case, the optimal solution depends on the choice of the initial stock. The reason is that the tank sizes s_p^M are influenced by the safety stock S_p^-, influencing not only the tank investment cost but also the storage cost.

In order to avoid artificially high storage costs, one can fix exactly one of the initial tank levels to the safety stock and leave the others variable, to be determined by the solution of the model. Recognize that fixing more then one tank level to the safety stock makes the problem infeasible.

Leaving all initial tank levels as free variables has the effect that the model will assign one of the tanks to the initial stock.

5. Properties of the Mathematical Model

In this section, we consider some properties of the mathematical model introduced in Section 4. We derive some useful properties when allowing empty campaigns, Section 5.1, we introduce some symmetry and sequence braking constrains, Section 5.2, we derive lower and upper bounds on the variables, Section 5.3, and we give an alternative mixed-integer programming formulation of the constraints, Section 5.4.

5.1. Allowing Empty Campaigns

Reflecting on constrains (12), we explicitly allow not assigning any product for a particular period n. This means together with constraints (18) that there is no production p_{pn}^{C} during that period. Furthermore, constraints (17) imply that the campaign length d_n is equal to zero. Hence, condition $\sum_{p \in \mathcal{P}} \omega_{pn} = 0$ can be interpreted as an empty campaign n.

The allowance of 'empty' campaigns has the following interesting property of the model. For any given (feasible) solution with N event points, we can 'extend' it to a feasible solution with $N + 1$ event points with the same objective function value by defining

$$\omega_{pN+1} = 0 \quad , \qquad \forall p \in \mathcal{P} \quad . \tag{31}$$

This implies that $d_{N+1} = 0$, $t_{N+1} = 0$, $p^{\mathrm{C}}_{pN+t} = 0$, $s_{pN+1} = s_{pN}$ for all products p and the cost per ton remain unchanged.

This leads directly to the following two corollaries.

Corollary 5.1. *Let $C^*(N)$ be the optimal cost per ton of the model dependent on the number of event points N. Then, $C^*(N)$ is a monotone decreasing function in N.*

Proof. The proof follows from the fact that any solution with N event points can be extended to a feasible solution with $N+1$ event points with the same objective function value. □

Recognize that Corollary 5.1 implicitly implies that the tank design problem is feasible for any $N \geq \overline{N}$, if it is feasible for $\overline{N}$.

Corollary 5.2. *Let N^* be an optimal number of event points for our model. Then, $N \geq N^*$ is also an optimal number of event points.*

Proof. From Corollary 5.1, we have that $C^*(N) \leq C^*(N^*)$ for all $N \geq N^*$ as $C^*(N)$ is monotone decreasing in N. As N^* is an optimal number of event points, $C^*(N) \geq C^*(N^*)$ which implies equality and the corollary is proven. □

Currently, we have no method how to compute N^*. However, when the objective function is not decreasing anymore with increasing number of event points, then Corollary 5.2 provides a practical way to stop the search for N^*.

5.2. Breaking Symmetry & Sequence

To destroy some symmetry and superfluous solutions we add the following constraints to the model

$$\sum_{p \in \mathcal{P}} \omega_{pn} \geq \sum_{p \in \mathcal{P}} \omega_{pn+1} \quad , \qquad \forall n \in \mathcal{N} \quad . \tag{32}$$

Constraints (32) shift the empty campaigns to the end of the planning horizon. In case that $\sum_{p \in \mathcal{P}} \omega_{pn} = 0$, the symmetry is broken and possible solutions with empty campaigns other than at the end of the planning horizon are eliminated.

Furthermore, with the allowance for empty constraints, we can add the following constraint to the model

$$1 - \omega_{pn} \geq \omega_{pn+1} \quad , \qquad \forall p \in \mathcal{P}, \quad \forall n \in \mathcal{N} \wedge n < N \tag{33}$$

We call constraints (33) sequence braking constraints, as they forbid the production of product p during event point $n+1$ if product p is produced during period n. Recognize that constraints (33) remove certain feasible solutions from the model but do not affect the optimal cost per ton $C^*(N)$.

We will observe the computational effectiveness of the symmetry braking constraints (32) and the sequence braking constraints (33) in Section 7.

5.3. Deriving Bounds on the Variables

The computational efficiency of global solvers depends crucially on the tightness of the upper and lower bounds on the variables. Some global solvers even require lower and upper bounds on all variables, *e.g.* BARON (32; 37).

As indicated in Section 4, some of the lower and upper bounds might not be given explicitly but have to be derived by other data; *for instance*, the lower and upper limit of the production amount.

The maximal length of a campaign is bounded by two processes: the capacity of a storage tank can be reached due to the continuous production, or the safety stock limit is reached due to the continuous sales of a product.

In the first case, if for a specific product p lower bounds on the production rates are provided or the production occurs at constant rates P_p^{R}, the maximal length of the campaigns is given by

$$D_p^{\mathrm{M_1}} := \frac{S_p^+ - S_p^-}{P_p^- - L_p} \quad ; \tag{34}$$

otherwise, *i.e.*, $D_p^{\mathrm{M_1}}$is set to $D_p^{\mathrm{M_1}} := +\infty$.

In the second case, we have

$$D_p^{\mathrm{M_2}} := \frac{S_p^+ - S_p^-}{L_p} \quad . \tag{35}$$

The upper bound on the campaign length for product p is then given by

$$D_p^+ := \min_p \left\{ D_p^{\mathrm{M_1}}, D_p^{\mathrm{M_2}} \right\} \quad . \tag{36}$$

These considerations also lead to the following remark. If P_p^- is too large, there are too large finite setup-change times T_p^S, and S_p^+ is very small, the problem may become easily infeasible.

5.4. An Equivalent Mixed-Integer Linear Formulation of the Constraints

Reflecting again the mathematical programming formulation of Section 4, we see that the only non-linear terms in the constraints are given by the trilinear terms $p^{\mathrm{R}}_{pn} d_n \omega_{pn}$ of constraints (18). In this section, we derive an equivalent mixed-integer linear programming formulation of that constraint introducing no additional constraints, leading to a linear constraint set of our tank design problem with integrality conditions.

With the bounds on the production rate given in constraints (19), we can eliminate the variable for the production rate, p^{R}_{pn}, and derive the equivalent inequalities

$$P^{R-}_{pn} d_n \omega_{pn} \leq p^{\mathrm{C}}_{pn} \leq P^{R+}_{pn} d_n \omega_{pn} \quad , \qquad \forall p \in \mathcal{P}, \quad \forall n \in \mathcal{N} \quad . \tag{37}$$

involving bilinear terms instead of trilinear ones.

Consider now the formal bilinear expressions

$$y_{pn} := d_n \omega_{pn} \quad , \qquad \forall p \in \mathcal{P}, \quad \forall n \in \mathcal{N} \quad . \tag{38}$$

The upper bound on the campaign length, D^{+}_{pn}, given in constraint (17), enables us to describe the variables y_{pn} by the following system of linear inequalities

$$\begin{aligned}
y_{pn} &\leq D^{+}_{pn} \omega_{pn} && , \qquad \forall p \in \mathcal{P}, \quad \forall n \in \mathcal{N} \quad , && (39)\\
y_{pn} &\leq d_n && , \qquad \forall p \in \mathcal{P}, \quad \forall n \in \mathcal{N} \quad , && (40)\\
y_{pn} &\geq d_n - D^{+}_{pn}(1-\omega_{pn}) && , \qquad \forall p \in \mathcal{P}, \quad \forall n \in \mathcal{N} \quad , && (41)\\
y_{pn} &\geq 0 && , \qquad \forall p \in \mathcal{P}, \quad \forall n \in \mathcal{N} \quad . && (42)
\end{aligned}$$

This formulation requires some comments. The case $\omega_{pn} = 0$ leads to $y_{pn} = 0$ via constraints (39) and (42), while $\omega_{pn} = 1$ generates the inequalities $y_{pn} \leq d_n$ and $y_{pn} \geq d_n$, *i.e.*, $y_{pn} = d_n$.

Hence, the variables y_{pn} are described via the mixed-integer linear constraints (39) - (42) and the bilinear constraints (38) will not enter the model explicitly. Notice that this formulation introduces $P \cdot N$ additional continuous variables to the model.

As we also have a lower bound on the campaign length, D^{-}_{pn}, via constraint (16), we are able to eliminate the auxiliary variables y_{pn} and derive the following system of linear inequalities

$$\begin{aligned}
P^{R-}_{pn} D^{-}_{pn} \omega_{pn} \leq p^{\mathrm{C}}_{pn} &\leq P^{R+}_{pn} D^{+}_{pn} \omega_{pn} && , \qquad \forall p \in \mathcal{P}, \quad \forall n \in \mathcal{N} \quad , && (43)\\
P^{R-}_{pn} \left(d_n - D^{+}_{pn} \left(1 - \omega_{pn}\right)\right) \leq p^{\mathrm{C}}_{pn} &\leq P^{R+}_{pn} d_n && , \qquad \forall p \in \mathcal{P}, \quad \forall n \in \mathcal{N} \quad . && (44)
\end{aligned}$$

For $\omega_{pn} = 0$, we get $p^{\mathrm{C}}_{pn} = 0$ through constraints (43). In case that $\omega_{pn} = 1$, constraints (44) come into play and result into the desired linear inequality

$$P^{R-}_{pn} d_n \leq p^{\mathrm{C}}_{pn} \leq P^{R+}_{pn} d_n \quad , \qquad \forall p \in \mathcal{P}, \quad \forall n \in \mathcal{N} \quad . \tag{45}$$

It is well known that the upper and lower bounds on d_n are crucial for the computational efficiency of the model. This is due to the reason that a common technique for optimization solvers for such type of problems is to relax the binary domain for the variables ω_{pn}, having the effect that the linear constraints (43) - (44) lead to a weaker formulation than constraints (37). Hence, one wants to make sure to derive as tight upper and lower bounds on d_n as possible.

6. Generalizations and Model Variations

In this section, we discuss two generalizations of the model presented in Section 4. Furthermore, a different approach for the tank investment modeling and a robust optimization model taking into account uncertain demand data are presented.

6.1. Sequence-Dependent Setup-Times

In practical planning processes in chemical plants, it often happens that the campaign setup-times of a product p depends heavily on the product $\overline{p}$ produced before; *i.e.*, it might take longer to clean the reactor when producing white color after black color than vise versa.

Therefore, let $T^{\mathrm{S}}_{\overline{p}p}$ [days] denote the sequence-dependent setup-times when producing product p directly after producing product $\overline{p}$. Then, we can change equation (14) to

$$t^{\mathrm{SC}}_n = \begin{cases} \sum_{p \in \mathcal{P}} T^{\mathrm{S}}_p \omega_{pn}, & \text{if } n = 1 \\ \sum_{\overline{p} \in \mathcal{P}} \sum_{p \in \mathcal{P}} T^{\mathrm{S}}_{\overline{p}p} \omega_{\overline{p}n-1} \omega_{pn}, & \text{if } n \neq 1 \end{cases} \tag{46}$$

with the initial setup time T^{S}_p when starting the production at the initial event point. Recognize that equation (46) involves the binary quadratic terms $\omega_{\overline{p}n-1}\omega_{pn}$ for $n > 1$ being equal to 1, if product $\overline{p}$ is produced at event point $n-1$ and product p is produced at event point n. Define

$$\lambda_{\overline{p}pn} := \omega_{\overline{p}n-1}\omega_{pn} \quad , \qquad \forall \overline{p}, p \in \mathcal{P}, \quad \forall n \in \mathcal{N} \quad , \tag{47}$$

then, expression (47) can be replaced by the following system of equations

$$\begin{aligned}
\lambda_{\overline{p}pn} &\leq \omega_{\overline{p}n-1} \quad , \qquad \forall \overline{p}, p \in \mathcal{P}, \quad \forall n \in \mathcal{N} \quad , && (48)\\
\lambda_{\overline{p}pn} &\leq \omega_{pn} \quad , \qquad \forall \overline{p}, p \in \mathcal{P}, \quad \forall n \in \mathcal{N} \quad , && (49)\\
\lambda_{\overline{p}pn} &\geq \omega_{\overline{p}n-1} + \omega_{pn} - 1 \quad , \qquad \forall \overline{p}, p \in \mathcal{P}, \quad \forall n \in \mathcal{N} \quad . && (50)
\end{aligned}$$

Hence, the bilinear terms in (46) can be expressed via three additional linear equations and one additional non-negative *continuous* variable for each of the $(N-1)P^2$ quadratic terms; see Kallrath and Wilson (24) for more details. This way, the number of binary variables and non-convex terms of the model remain the same.

6.2. Multiple Reactors

In this section, we present a model having mainly three additional features to the single reactor case: It generalizes to multiple reactors, idle reactor time is allowed and the same product can be produced in two proceeding event points while a change of the production rate is possible.

A natural way to extend the presented model to the case of multiple reactors is to replace the binary variables ω_{pn} by

$$\omega_{pnr} = \begin{cases} 1, & \text{if product } p \text{ is produced at reactor } r \text{ during time period } n \\ 0, & \text{otherwise} \end{cases} \quad , \tag{51}$$

with $r \in \mathcal{R} := \{1, 2, \ldots, R\}$ being the set of $R(\geq 2)$ reactors. The idea is to synchronize the decisions for all reactors; *i.e.*, to allow a mode change for each reactor at the same event point. In order to allow mode changes at any given time, one has to ensure that the products can be produced at proceeding periods.

Let us now have a look at the constraints of the model of Section 4 to make the necessary adjustments. In the multiple reactor case, exactly one product has to be produced on each reactor at each event point

$$\sum_{p \in \mathcal{P}} \omega_{pnr} = 1 \quad , \qquad \forall n \in \mathcal{N}, \quad \forall r \in \mathcal{R} \quad . \tag{52}$$

Empty campaigns and/or reactor idle times can be modeled by adding a dummy product with zero demand. This way, also Corollary 5.1 and Corollary 5.2 hold true for the multiple reactor model.

The cycle time T is still given by (13). However, the length of each period and campaign is no longer given by equations (15) but instead determined through the following system of constraints:

$$d^+_{nr} - d^-_{nr} = t_n - t^{\mathrm{SC}}_{nr} - d^-_{n-1r} \quad , \qquad \forall n \in \mathcal{N}, \quad \forall r \in \mathcal{R} \quad , \tag{53}$$

$$d^-_{n-1r} \leq \left(D^+_{pn} + T^{\mathrm{S}}_p\right) \cdot (1 - \delta_{pnr}) \quad , \qquad \forall n \in \mathcal{N}, \quad \forall r \in \mathcal{R}, \quad \forall r \in \mathcal{R} \tag{54}$$

$$d^-_{Nr} = 0 \quad , \qquad \forall r \in \mathcal{R}, \tag{55}$$

$$d^+_{nr},\, d^-_{nr} \geq 0 \quad , \qquad \forall n \in \mathcal{N}, \quad \forall r \in \mathcal{R}, \tag{56}$$

with the convention $d^-_{0r} \equiv 0$ and the binary variables δ_{pnr} indicating if the production of product p starts at the beginning of period n, *i.e.*,

$$\delta_{p1r} \;=\; (1 - \omega_{pNr})\, \omega_{p1r} \quad , \qquad \forall p \in \mathcal{P}, \quad \forall r \in \mathcal{R} \quad , \tag{57}$$

$$\delta_{pnr} \;=\; (1 - \omega_{pn-1r})\, \omega_{pnr} \quad , \qquad \forall p \in \mathcal{P}, \quad \forall n \in \mathcal{N}, \quad \forall r \in \mathcal{R} \quad , \tag{58}$$

and the setup-times in (14) extend to the multiple reactors case as

$$t^{\mathrm{SC}}_{nr} = \sum_{p \in \mathcal{P}} T^{\mathrm{S}}_p \delta_{pnr} \quad , \qquad \forall n \in \mathcal{N}, \quad \forall r \in \mathcal{R} \quad . \tag{59}$$

Recognize that through equations (54), (57) and (58), at most one of the variables t^{SC}_{nr} and d^-_{n-1r} is positive for any pair n and r. Hence, variable d^+_{nr} is the production length of period n on reactor r and d^-_{nr} transfers the remaining setup-time to the next period $n+1$. With positive variable storage cost $C^{\mathrm{S}}_p > 0$, relation $d^+_{nr} d^-_{nr} = 0$ is ensured most of the time. As there may be no production during the setup-time, it might be that both variables d^+_{nr} and d^-_{nr} are positive at the same time. This could be the case if the whole duration of the event point t_n is smaller than the setup-time, this particular product has no production during that time on one of the other reactors and the stock of this product is at its minimum. Forcing one of the two variables d^+_{nr} and d^-_{nr} to have a zero value would make such a schedule infeasible, while our model allows to 'borrow' some production time from the next period and to give it 'back' afterwards. The consequence is a slight inaccuracy in the storage cost, however, this is consistent with the simplifications made in equations (27).

The variables δ_{p1r} for the first period defined in (57) capture the cyclic effect of the lot-sizing problem; *i.e.*, if a product is produced in the last period of the planning horizon, then the production of this product does not 'start' in period 1 and no setup-time and setup-cost are required. The bilinear terms in (57) and (58) can be linearized in a straight forward manner; *cf.* Section 6.1.

To ensure semi-continuous lower bounds D^-_{pn} on the lengths of each production, we replace (16) by the following system of constraints

$$d^+_{nr} + d^\times_{nr} \geq \sum_{p\in\mathcal{P}} D^-_{pn}\delta_{pnr} + d^\times_{n-1r} \quad , \qquad \forall n \in \mathcal{N}, \quad \forall r \in \mathcal{R} \quad , \tag{60}$$

$$d^\times_{n-1r} \leq \left(D^+_{pn} + T^\mathrm{S}_p\right)\cdot(1-\delta_{pnr}) \quad , \qquad \forall p \in \mathcal{P}, \quad \forall n \in \mathcal{N}, \quad \forall r \in \mathcal{R} \tag{61}$$

$$d^\times_{Nr} = 0 \quad , \qquad \forall r \in \mathcal{R}, \tag{62}$$

$$d^\times_{nr} \geq 0 \quad , \qquad \forall n \in \mathcal{N}, \quad \forall r \in \mathcal{R} \quad , \tag{63}$$

with $d^\times_{0r} \equiv 0$. In a similar way, the constraints on semi-continuous upper bounds in (17) can be modeled.

The production during each period depends now also on the reactor; equation (18) is replaced by

$$p^\mathrm{C}_{pn} = \sum_{r\in\mathcal{R}} p^\mathrm{C}_{pnr} \quad , \quad \forall p \in \mathcal{P}, \quad \forall n \in \mathcal{N} \quad , \tag{64}$$

and

$$p^\mathrm{C}_{pnr} = p^\mathrm{R}_{pnr} d^+_{nr}\omega_{pnr} \quad , \qquad \forall p \in \mathcal{P}, \quad \forall n \in \mathcal{N}, \quad \forall r \in \mathcal{R} \quad . \tag{65}$$

The constraints on the production rate (19) as well as the semi-continuous lower bounds (20) and upper bounds (21) hold also true for each reactor r. The definition of the production rate in equation (65) allows that the same product can be produced in proceeding event points where the production rate can change. If the production rate has to stay constant throughout the whole production period, then one may couple the variables p^C_{pnr} with ω_{pnr}.

With equations (57) and (58), the campaign setup cost are calculated via

$$c^\mathrm{C} = \sum_{p\in\mathcal{P}} \sum_{n\in\mathcal{N}} \sum_{r\in\mathcal{R}} C^\mathrm{C}_p \delta_{pnr} \quad . \tag{66}$$

All other cost terms (4), (5), (11), (28), as well as (29) remain unchanged along with relations (22), (23) and (24).

6.3. Discrete Tank Sizes

Large tanks can be ordered at any size while small tanks are usually given with pre-defined tank sizes. In order to allow to choose from a discrete set of different tanks for each product, we introduce the binary variables

$$\delta_{p\tau} = \begin{cases} 1, & \text{if tank } \tau \text{ is installed for product } p \\ 0, & \text{otherwise} \end{cases} \quad , \tag{67}$$

with $\tau \in \mathcal{T}_p$ being the set of possible tanks with capacity $S^+_{p\tau}$ for product $p \in \mathcal{P}$. Let $c^{\mathrm{I}}_{p\tau}$ [\$/day] be the tank investment cost scaled to one day for tank $\tau \in \mathcal{T}_p$ and product $p \in \mathcal{P}$. Then, the tank investment costs of equation (5) can be replaced by

$$c^{\mathrm{I}} = \sum_{p \in \mathcal{P}} c^{\mathrm{I}}_{p\tau} \delta_{p\tau} \quad . \tag{68}$$

As we only allow exactly one tank per product p, we need the constraint

$$\sum_{\tau \in \mathcal{T}_p} \delta_{p\tau} = 1, \qquad \forall p \in \mathcal{P} \quad . \tag{69}$$

The bounds on the tank filling levels are then given by

$$\sum_{\tau \in \mathcal{T}_p} \delta_{p\tau} S^-_{p\tau} \leq s_{pn} \leq \sum_{\tau \in \mathcal{T}_p} \delta_{p\tau} S^+_{p\tau} \quad , \qquad \forall p \in \mathcal{P}, \quad \forall n \in \mathcal{N} \tag{70}$$

which replaces constraints (23).

The discrete model of the tank sizes removes the concave function $f(s^M_p, p)$ from equation (5) and the problem becomes a non-convex mixed-integer quadratic constraint programming problem. However, additional $|\mathcal{T}_p|$ bilinear terms are added to the objective function expression (11) as the cycle time T is unknown.

For computational reasons it is better to replace the binary restriction on the variables $\delta_{p\tau}$ by Special Order Set of type 1 (SOS-1), as at most one variable of this set can have a nonzero value. The concept of SOS-1 was introduced by Beale and Tomlin (1). For more details on SOS-1 sets, we refer to Kallrath and Wilson (24, Chapter 6.7) and Kalvelagen (25).

6.4. Two Stage Stochastic Programming Approach for Demand Uncertainty

The major drawback of the presented model is that it neglects that the daily demands L_p for each product p are uncertain. More realistic is to assume that the demand varies between certain bounds or that we are given different possible scenarios for the demand; *i.e.*, one scenario could be to assume that there will be an economy boom leading to a high daily demand.

Given that the demand for each product is uncertain, we want to find an investment decision for the storage tanks which leads to a feasible solution for all different demand scenarios – hence, we want the tank investment decision to be *robust* with respect to the demand uncertainty.

Robust optimization approaches for scheduling problems under demand uncertainty following the ideas of Lin et al. (29) would use the upper bound on the daily demand value (minus a pre-defined infeasibility tolerance) to determine a production schedule. However, in our problem, we do not only want that the tank investment decisions can deal with the worst case, but we also want to minimize the *expected* cost, that is, the tank investment cost plus the *expected* operational cost. This can be modeled as a two stage stochastic program where the first stage decisions represent the tank investment decisions and the recurse decisions are the operational decisions. This way, the investment decision in a tank has to be made before the actual demand is known. After the tank has been installed, a certain demand scenario is going to occur and the production can be scheduled.

Therefore, let $\mathcal{S} := \{1, 2, \ldots, S\}$ be the set of S possible scenarios with demand L_{ps} for each product $p \in \mathcal{P}$ and scenario $s \in \mathcal{S}$ having probability Pr_s. Obviously, we have

$$\sum_{s \in \mathcal{S}} Pr_s = 1 \quad . \tag{71}$$

Then, all operational decisions depend on the demand scenarios $s \in \mathcal{S}$. Hence, there are S copies for each of the variables modeling the scheduling problem; *i.e.*, denoted by the variables p^{C}_{pns}, p^{T}_{s}, s_{pns}, t_{ns}, d_{ns}, t^{SC}_{ns}, T_s, ω_{pns}, and s^{H}_{pns} for all $p \in \mathcal{P}$, $n \in \mathcal{N}$ and $s \in \mathcal{S}$. Recognize that the variables s^{M}_{p} modeling the size of the design tanks are independent of the scenarios, representing the first stage decision.

Consistent with equation (10), we define the total demand per day for scenario $s \in \mathcal{S}$ as

$$L_s := \sum_{p \in \mathcal{P}} L_{ps} \quad . \tag{72}$$

By substituting the appropriate variables, let for each scenario $s \in \mathcal{S}$ the campaign setup cost be c^{C}_{s} corresponding to (66), the variable production cost be c^{P}_{s} corresponding to (4), and the storage cost be c^{S}_{s} corresponding to (29).

Then, the *operational* cost per ton, c_s^{OPT}, for scenario s can be derived through relation

$$c_s^{\mathrm{OPT}} T_s L_s = c_s^{\mathrm{C}} + c_s^{\mathrm{P}} + c_s^{\mathrm{S}} \quad , \tag{73}$$

where the variable production costs c_s^{P} is a constant for c_s^{OPT}; just like in the deterministic case. Together with the tank investment cost per ton produced, this leads to the objective function

$$\frac{1}{365H[\text{days/year}]} \left(\sum_{p \in \mathcal{P}} f(s_p^M, p) \right) \left(\sum_{s \in \mathcal{S}} \frac{Pr_s}{L_s} \right) + \sum_{s \in \mathcal{S}} Pr_s c_s^{\mathrm{OPT}} \quad , \tag{74}$$

being minimized. Equation (74) represents the expected cost per ton.

The constraints on the amount of product stored in the tanks are given by

$$S_p^- \leq s_{pns} \leq s_p^M \leq S_p^+ \quad , \qquad \forall p \in \mathcal{P}, \quad \forall n \in \mathcal{N}, \quad \forall s \in \mathcal{S} \quad , \tag{75}$$

which substitutes equation (23). All other constraints (12), (13), (14), (15), (16), (17), (18), (19), (20), (21), (22), (24) and (28) have to hold true for each scenario $s \in \mathcal{S}$. Recognize that these constraints are only connected via equation (75).

Compared to the deterministic model, the two stage stochastic model proposed increases the number of variables and constraints significantly (roughly by a multiplier of S). However, even more crucial are the additional non-convex terms.

7. Computational Results

The mathematical programming formulation described in Section 4 is a MINLP formulation due to the non-convex objective function and the binary variables to decide which product has to be produced in each campaign. Therefore, we need global optimization techniques to compute the global optimum.

The mathematical program is implemented in the modeling language GAMS, version 23.2.1. The code has been added to the GAMS model library under the name `tanksize` (GAMS). The MINLP problem is solved with the global solvers BARON (37, version 8.1.5) and LINDOGlobal (30,

N	c^{PT}						GAP		CPU					
	AE	CB	DI	SB	BA	LG	BA	LG	AE	CB	DI	SB	BA	LG
3	1.269	1.269	–	–	1.269	1.269	0.00%	0.00%	0:00:55	0:00:01	0:00:01	0:00:01	0:00:14	0:00:04
4	1.269	1.269	–	–	1.269	1.269	0.00%	0.00%	0:00:54	0:00:05	0:00:01	0:00:01	0:45:45	0:00:30
5	1.257	1.257	–	–	1.257	1.257	19.04%	0.00%	0:00:30	0:00:11	0:00:01	0:00:01	‡	0:01:51
6	1.257	1.257	–	–	1.257	1.257	23.72%	0.00%	0:00:36	0:00:29	0:00:01	0:00:01	‡	0:05:49
7	1.257	1.257	–	–	1.257	1.257	26.64%	0.00%	0:00:36	0:00:53	0:00:01	0:00:01	‡	0:14:56
8	1.269	1.257	–	–	1.257	1.257	30.05%	0.00%	0:00:42	0:01:57	0:00:01	0:00:01	‡	0:57:35

– No feasible solution found.

‡ Time limit of 5h was reached.

Table 1: Computational results for three products comparing different MINLP solvers.
Nonlinear solvers: Alpha-ECP (AE), CoinBonmin (CB), Dicopt (DI), SBB (SB)
Global solvers: BARON (BA), LINDOGlobal (LG)

version 5.0.1.183) as well as with the nonlinear solvers Alpha-ECP (39, version 1.75.03), CoinBonmin (2, version 1.0), Dicopt (7, version 2x-C), and SBB (12). The standard settings for all solvers are used. The operation system is Windows XP and the computational tests are done on a Intel Pentium Centrino Dual 2.00 GHz with 1GB RAM, where only one processor is used in order to be able to repeat the computational tests.

Some computational results for three products (one reactor and sequence-independent campaign setup-times) are given in Table 1. N is the number of event points, given as input data for the solver; c^{PT} states the cost per ton, excluding the variable production cost as well as the fixed part of the tank investment cost; the optimality gap (GAP) is calculated as the difference of the upper bound and the lower bound divided by the upper bound; the CPU time is given in h:mm:ss. All instances where solved with six different MINLP solvers. We observe that Alpha-ECP and CoinBonmin are able to find the global optimum (except for one instance) while Dicopt and SBB do not find a feasible solution. The computational time to prove global optimality for a fixed number of event points N increases significantly with N for LINDOGlobal. BARON was not able to close the gap for $N \geq 5$ – let us point out again that only the standard settings were used.

Even for the relative small instance with three products, we are not able to prove that the solution found is globally optimal with respect to N, *i.e.*, the cost per ton is minimal over all event points. However, due to the model structure discussed in Section 5.1, $N = 5$ looks like a good candidate for the global optimum, as the cost per ton do not decrease while increasing N

N	T	s_1^M	s_2^M	s_3^M	P_1	P_2	P_3	c^{PT}
3, 4	11.316	682.779	621.633	253.101	1	2	3	1.269
5, 6, 7, 8	17.048	678.605	594.598	273.872	1, 3	2, 5	4	1.257

Table 2: Optimal solutions for three products corresponding to the results of Table 1.

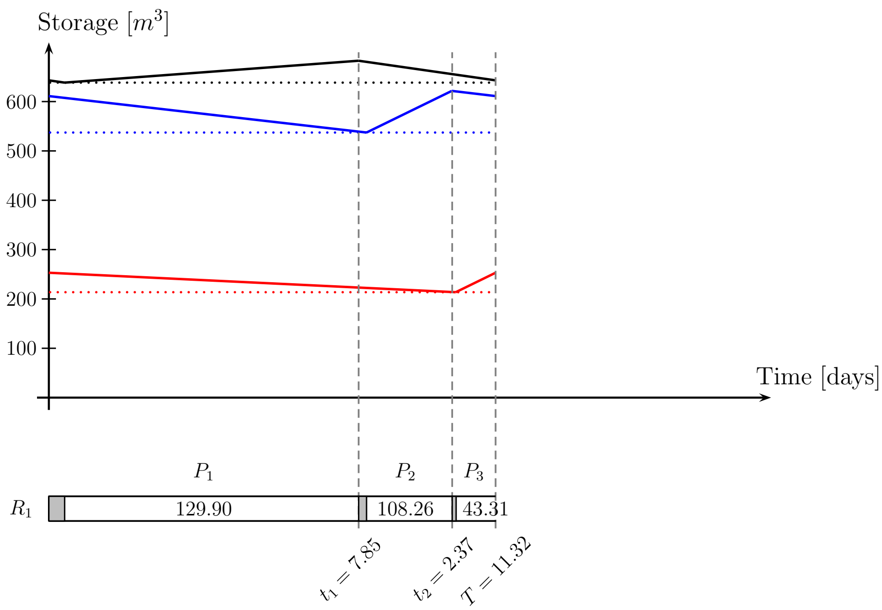
further.

Optimal solutions for the instances tested in Table 1 are presented in Table 2. T is the optimal cycle time for given N, s_p^M are the tank sizes for each of the three products $p \in \mathcal{P} = \{1, 2, 3\}$. The periods where each product p is scheduled for is given in the columns P_p. The corresponding optimal solution for three products and $3 \leq N \leq 8$ event points is shown in Figure 4. The tank storage levels for the three tanks over the planning horizon T are shown on top of a Gantt chart. Consistent with Figure 3, the gray shaded areas indicate the setup-times and the production rates are given in the Gantt charts. Interestingly, the optimal solution for the case of 3 and 4 event points is the same while the optimal cost per ton decreases when $N = 5$.

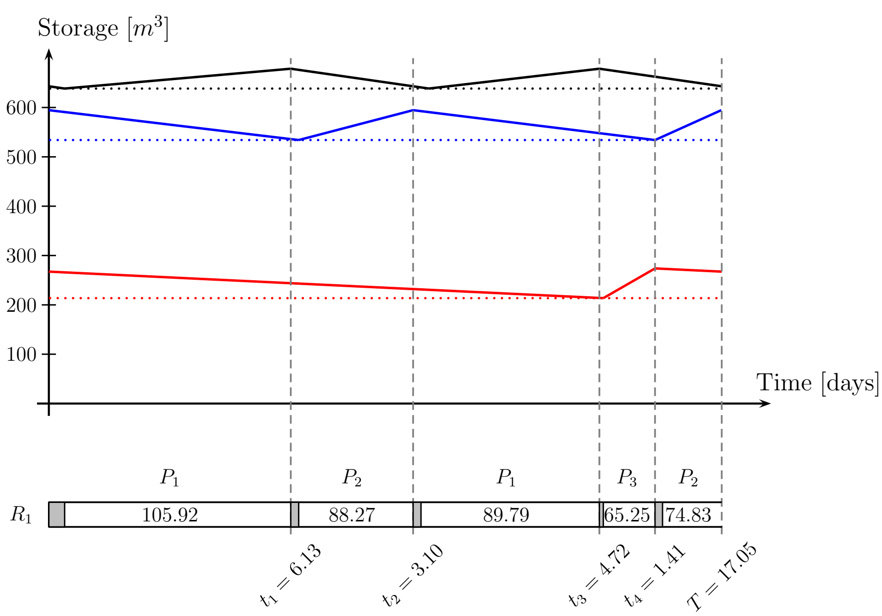
Table 3 shows the effects of the symmetry braking constraints (32) and the sequence braking constraints (33) discussed in Section 5.2. Column 'Sol.' gives the number of (box) iterations for LINDOGlobal until the optimal solution is found whereas 'Total' provides the number of iterations until global optimality is proven. While the running time and the number of iterations are similar for $3 \leq N \leq 5$, significant computational differences for all four cases for $6 \leq N \leq 8$ are observed. Recognize that for $N \geq 6$ many alternative optimal solutions exists as the optimal objective function value is the same as for $N = 5$ and this is where the additional constraints (32) and (33) show their efficiency. Optimal solutions where found by LINDOGlobal with relatively few iterations. Hence, the time consuming part is the computation of the bounds and this is where the symmetry and sequence braking constraints help.

Table 4 summarizes some computational results for four products. The following observations seem to be most important:

- for fixed number of event points, global optimality cannot be proven within 5 hours for $N \geq 8$;
- to find the optimal solution for fixed number of event points is a much



(a) $3 \leq N \leq 4$



(b) $5 \leq N \leq 8$

Figure 4: Optimal solutions for three products and different number of event points N corresponding to Table 2.

	with Symmetry & with Sequence			with Symmetry & Sequence broken (33)			Symmetry broken & with Sequence (32)			Symmetry broken & Sequence broken (33) & (32)		
N	# Iterations		CPU	# Iterations		CPU	# Iterations		CPU	# Iterations		CPU
	Sol.	Total		Sol.	Total		Sol.	Total		Sol.	Total	
3	3	62	0:00:05	0	61	0:00:05	3	63	0:00:04	2	61	0:00:04
4	0	521	0:00:37	0	507	0:00:34	0	396	0:00:28	110	368	0:00:29
5	2	1719	0:03:15	0	1692	0:03:01	9	1477	0:03:42	0	1001	0:01:51
6	4	9134	0:19:49	6	7647	0:16:24	5	2901	0:09:52	2	2065	0:05:49
7	37	34606	1:32:42	9	27751	1:10:36	0	7707	0:31:26	28	4553	0:14:56
8	121	134320	7:40:43	5	106632	5:49:11	85	26358	2:00:29	2	15480	0:57:35

Table 3: Computational results for LINDOGlobal with and without sequence braking constraints (33) and with and without symmetry braking constraints (32).

more challenging task than in the case of three products, which can be seen by the increase in computational time and by the fact that the nonlinear solvers do not always find the global optimum;

- the optimal number of event points seems to be much larger than for the case of three products.

Table 5 summarizes the best solutions found for each event point corresponding to the four product case of Table 4. At a first glance, it might be surprising that the optimal cycle time T does not change for $3 \leq N \leq 10$. The reason is that the yearly demand for product four is 78 tons, while the minimum production period D_4^- is 1 day and the minimum production rate $P_4^{\mathrm{R}-}$ is 7.00, leading to a minimal cycle time T of 32.756. Solutions for some event points are shown in Figure 5.

7.1. Model Variations

Let us now discuss the effects of the generalizations and model variations of Section 6.

We take the case of three products of Table 1 where the setup-times are changed to be sequence-dependent as follows: the change from P1 to P2 takes now 75% longer and the change from P2 to P1 takes half of the time as before. All other setup-times remain the same. The corresponding optimal solutions and the computational time for LINDOGlobal are shown in Table 6. One observes that the running times are similar to the case with sequence-independent setup-times.

N	c^{PT}						GAP		CPU					
	AE	CB	DI	SB	BA	LG	BA	LG	AE	CB	DI	SB	BA	LG
4	1.659	1.659	–	–	1.659	1.659	0.00%	0.00%	0:04:14	0:00:06	0:00:01	0:00:01	0:05:28	0:00:10
5	1.577	1.577	1.630	1.577	1.577	1.577	28.44%	0.00%	1:43:20	0:00:48	0:00:02†	0:00:14	‡	0:02:47
6	1.459	1.459	–	1.459	1.468	1.459	31.47%	0.00%	0:38:27	0:01:44	0:00:01	0:00:46	‡	0:15:50
7	1.435	1.413	–	1.413	1.440	1.413	32.38%	0.00%	0:40:50	0:04:35	0:00:03†	0:01:07	‡	1:35:08
8	1.413	1.403	–	1.403	1.483	1.403	36.34%	9.94%	0:35:09	0:11:10	0:00:01	0:01:29	‡	‡
9	1.371	1.371	–	1.371	–	1.371	–	18.73%	‡	0:23:09	0:00:03†	0:02:41	‡	‡
10	1.459	1.366	–	–	–	1.366	–	23.62%	2:26:08	1:25:02	0:00:01	0:00:01	‡	‡
11	1.416	1.362	–	1.362	–	1.362	–	25.80%	0:56:28	3:23:02	0:00:03†	0:09:26	‡	‡
12	1.413	1.364	–	1.362	–	1.362	–	27.37%	2:56:16	‡	0:00:01	0:24:45	‡	‡
13	1.428	1.360	1.418	–	–	1.359	–	28.71%	0:33:26	‡	0:00:08†	0:00:01	‡	‡
14	1.374	1.359	1.418	1.360	–	1.359	–	30.17%	1:46:35	‡	0:00:09†	0:18:30	‡	‡
15	1.367	1.359	1.418	–	–	1.359	–	31.01%	0:01:20	‡	0:00:09†	0:12:41	‡	‡

– No feasible solution found.

† Execution was stopped due to solver problems.

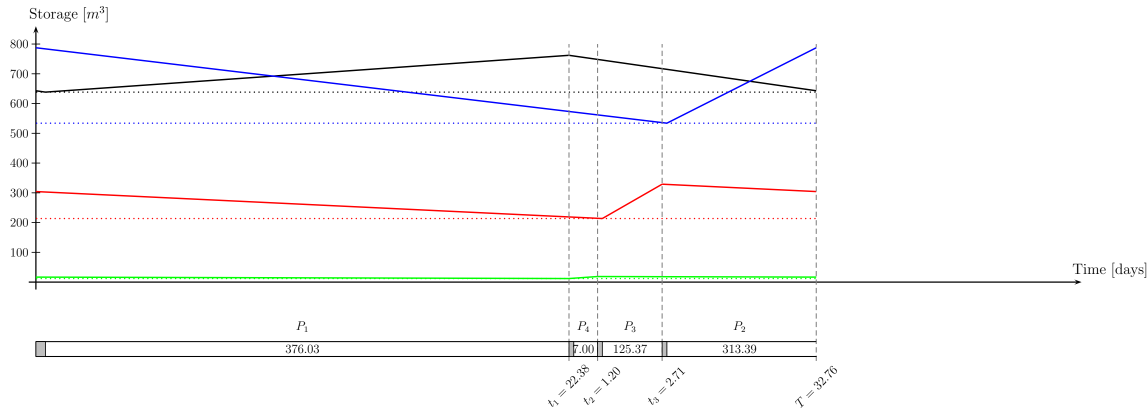
‡ Time limit of 5h was reached.

Table 4: Computational results for four products comparing different MINLP solvers.
Nonlinear solvers: Alpha-ECP (AE), CoinBonmin (CB), Dicopt (DI), SBB (SB)
Global solvers: BARON (BA), LINDOGlobal (LG)

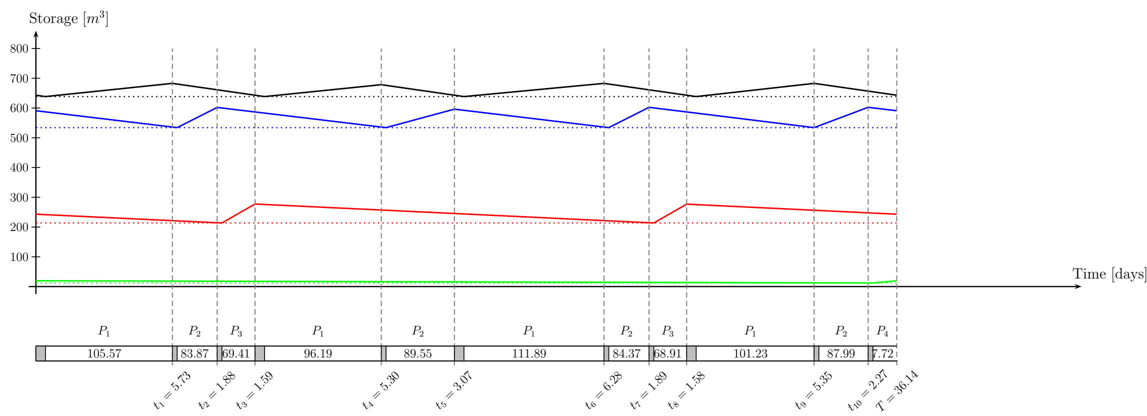
N	T	s_1^M	s_2^M	s_3^M	s_4^M	P_1	P_2	P_3	P_4	c^{PT}
4	32.756	762.101	787.507	329.009	18.744	1	4	3	2	1.659
5	32.756	809.221	710.854	305.859	18.744	1, 4	5	2	3	1.577
6	32.756	710.695	654.966	329.009	18.744	1, 4	2, 5	3	6	1.458
7	32.756	711.185	657.573	272.595	18.744	1, 5	2, 6	3, 7	7	1.413
8	32.756	701.605	659.884	278.081	18.744	1, 3, 6	2, 5	4, 8	7	1.403
9	32.756	697.736	609.406	273.506	18.744	1, 5, 7	2, 6, 9	4, 8	3	1.371‡
10	32.756	684.057	611.969	611.969	18.744	1, 3, 6, 8	2, 4, 7	5, 10	9	1.371‡
11, 12	36.141	682.783	602.311	277.335	19.467	1, 4, 6, 9	2, 5, 7, 10	3, 8	11	1.362‡
13, 14, 15	42.890	685.444	610.174	262.310	20.909	1, 3, 6, 9, 11	2, 5, 7, 10	4, 8, 12	13	1.359‡

‡ Global optimality could not be proven within 5h.

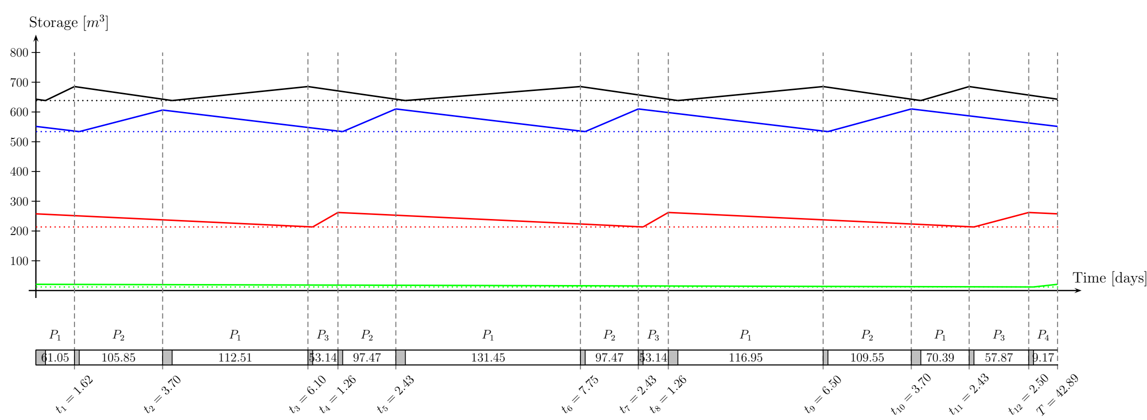
Table 5: Good solutions for four products corresponding to the results of Table 4.



(a) $N = 4$



(b) $11 \leq N \leq 12$



(c) $13 \leq N \leq 15$

Figure 5: Good solutions for four products and different number of event points N corresponding to Table 5.

N	T	s_1^M	s_2^M	s_3^M	P_1	P_2	P_3	c^{PT}	CPU
3	11.314	689.663	616.835	252.711	1	2	3	1.271	0:00:04
4	12.902	706.331	606.654	248.175	1, 3	2	4	1.269	0:00:34
5	17.046	681.715	593.431	272.717	1, 4	3, 5	2	1.258	0:02:19
6	17.046	681.715	593.431	272.717	1, 4	3, 5	2	1.258	0:05:28
7	17.046	681.715	593.431	272.717	1, 4	3, 5	2	1.258	0:12:40
8	17.046	681.715	593.431	272.717	1, 4	3, 5	2	1.258	0:52:32

Table 6: Computational results for three products with sequence-dependent setup-times using the solver LINDOGlobal.

Recall that the model for multiple reactors involves not only additional binary decision variables for each reactor r defined in (51), but also complicating constraints such as in (53) - (61). This makes it already difficult to find a feasible solution, while proving optimality is an even more challenging task. This can be observed in Table 7 where a case of two reactors and four products with an additional dummy product having zero demand is shown. For the sequencing decision, the reactor number and the period numbers are shown; *i.e.*, 'R2-3' means that reactor two during period three is used. One observes that the cost per ton decreases significantly compared to the single reactor case; even when allowing the double number of event points for the single reactor case. This is due to the decrease in the tank investment cost and the tank storage cost. Interestingly, the case with two event points is infeasible for this instance due to the minimum production rates and the minimum duration for each production period.

The corresponding solutions for the two reactor case are presented in Table 8 and are shown in Figure 6. The solution details for $N = 7$ event points are not presented, as the cost per ton are higher than for the case of $N = 4, 5$, and 6 event points which means that this solution cannot be optimal; *cf.* Section 6.2. Consider now the solution for $N = 3$ event points. We observe that reactor one is idle during period two in the optimal solution and that product 3 is produced during period two and three on reactor two, where a change in the production rate at $n = 2$ occurs.

Consider now Table 9. Computational results are presented for the case of discrete tank investment decisions as discussed in Section 6.3. As the upper bound on the tank sizes are relatively large for the computational tests presented in Table 1 and Table 2, we divide the upper bound first by five and then use a uniform discretization with 1, 3, 5 or 10 steps; we use the same

N	c^{PT}						GAP		CPU					
	AE	CB	DI	SB	BA	LG	BA	LG	AE	CB	DI	SB	BA	LG
3	1.431	–	–	–	1.431	1.431	0.00%	0.00%	0:18:44	0:00:01†	0:00:01	0:00:01	3:12:09	0:01:17
4	1.360	–	–	–	1.376	1.350	28.81%	27.37%	2:39:30	0:00:01†	0:00:01	0:00:01	‡	3:39:11†
5	1.329	–	–	–	1.385	1.317	33.87%	30.78%	‡	0:00:01†	0:00:01	0:00:01	‡	‡
6	1.319	–	–	–	1.556	1.317	42.23%	32.04%	‡	0:00:01†	0:00:01	0:00:01	2:47:36†	‡
7	1.320	–	–	–	1.377	1.357	35.44%	34.63%	‡	0:00:01†	0:00:01	0:00:01	‡	‡

– No feasible solution found.

† Execution was stopped due to solver problems.

‡ Time limit of 5h was reached.

Table 7: Computational results for four products and two reactors comparing different MINLP solvers.

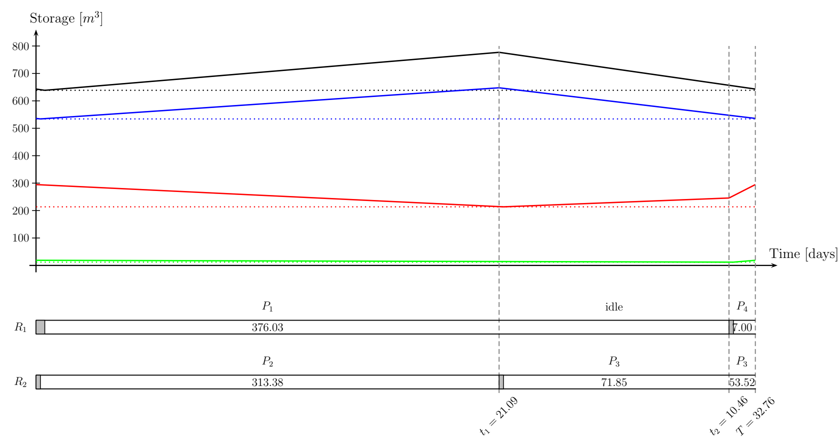
Nonlinear solvers: Alpha-ECP (AE), CoinBonmin (CB), Dicopt (DI), SBB (SB)

Global solvers: BARON (BA), LINDOGlobal (LG)

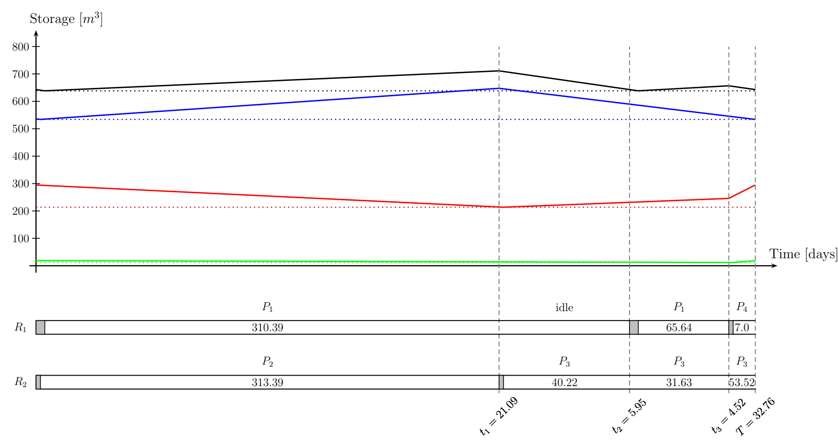
N	T	s_1^M	s_2^M	s_3^M	s_4^M	P_1	P_2	P_3	P_4	c^{PT}
3	32.756	776.898	647.592	294.729	18.744	R1-1	R2-1	R1-3, R2-2	R2-3	1.432
4	32.756	711.256	647.592	294.729	18.744	R1-1, R1-3	R2-1	R2-2, R2-3, R2-4	R1-4	1.350‡
5, 6	32.756	684.063	667.072	278.856	18.744	R1-1, R2-3	R2-1, R2-2	R1-3, R1-4, R1-5	R2-4	1.317‡

‡ Global optimality could not be proven within 5h.

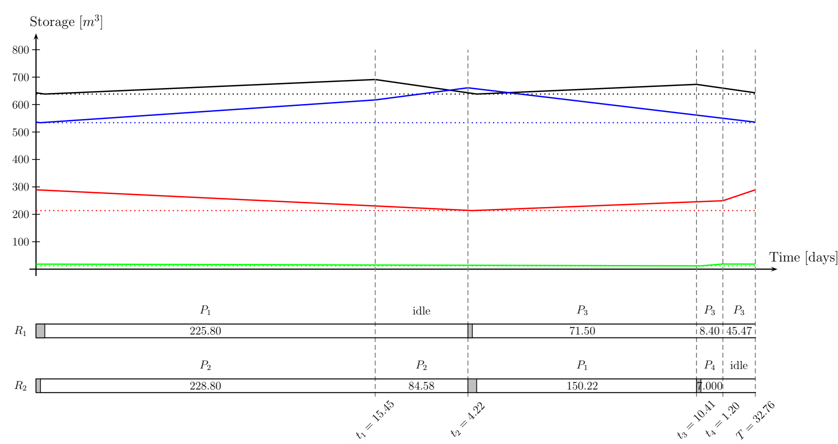
Table 8: Computational results for two reactors and four products computed with LINDOGlobal.



(a) $N = 3$



(b) $N = 4$



(c) $5 \leq N \leq 6$

Figure 6: Good solutions for two reactors and different number of event points N corresponding to Table 8.

discretization size for the tanks of each product. The case of 1 discretization of the tank capacity is a pure lot-sizing problem with non-linear storage cost. Observe that the computational efficiency decreases dramatically when increasing the size of $\mathcal{T}_p$. Comparing the computational performance with the case of continuous tanks sizes is sobering. It seems that the additional binary variables in the objective function make it more difficult to compute tight bounds. Hence, a discrete model should only be used if implied by practice or when a very good approximation of the optimal storage size is known as the computational time as well as the cost per ton are worse than for the case of continuous tank sizes.

Table 10 shows the optimal solutions for each of the cases presented in Table 9. Most the time, the sequencing decisions remain the same for different tank discretizations and the same number of event points. The solutions for five event points with $|\mathcal{T}_p| = 5$ and $|\mathcal{T}_p| = 10$ show that there are different optimal cycle times T while having the same sequencing decision and the same tank sizes. For the case of $|\mathcal{T}_p| = 10$, the cost per ton for three and four event points do not change, while the optimal cycle time and the sequencing decisions differ. The solution with $N = 4$ is slightly better ($\approx 0.036\%$).

N	c^{PT}				CPU			
	$\lvert\mathcal{T}_p\rvert = 1$	$\lvert\mathcal{T}_p\rvert = 3$	$\lvert\mathcal{T}_p\rvert = 5$	$\lvert\mathcal{T}_p\rvert = 10$	$\lvert\mathcal{T}_p\rvert = 1$	$\lvert\mathcal{T}_p\rvert = 3$	$\lvert\mathcal{T}_p\rvert = 5$	$\lvert\mathcal{T}_p\rvert = 10$
3	1.313	1.276	1.275	1.271	0:00:03	0:00:42	0:02:10	0:05:32
4	1.311	1.273	1.272	1.271	0:00:42	0:05:46	0:11:41	0:23:07
5	1.305	1.262	1.260	1.260	0:01:42	0:15:04	0:27:01	2:19:39
6	1.305	1.262	1.260	1.260	0:04:35	0:26:36	1:54:17	7:42:52

Table 9: Computational results for LINDOGlobal with discrete tank sizes for three products.

Similar to the case of multiple reactors, the two stage stochastic programming approach for demand uncertainty introduced in Section 6.4 increases the problem size significantly. We can observe this also in the computational results shown in Table 11. Three different demand scenarios with equal probability are considered, with the ‘normal’ demand scenario corresponding to the case of Table 1, the ‘high’ demand scenario has an increase of 20% in demand and the ‘low’ demand scenario has a demand decrease of 10%. For a given number of event points N, the computational results for LINDOGlobal along with the solutions are presented in each row where the ‘case’ value in the second column reads ‘stochastic’. For each of the three scenarios, the optimal cycle time T_s is shown. Remember that the optimal investment

N	$\vert\mathcal{T}_p\vert$	T	s_1^M	s_2^M	s_3^M	P_1	P_2	P_3	c^{PT}
3	1	12.826	803.672	669.726	267.890	1	2	3	1.313
3	3	10.487	696.557	625.151	249.927	1	2	3	1.276
3	5	12.252	707.269	616.236	257.112	1	3	2	1.275
3	10	10.956	691.202	616.236	251.723	1	2	3	1.271
4	1	14.763	803.672	669.726	267.890	$1,3$	4	2	1.311
4	3	13.317	696.557	625.151	249.927	$1,3$	4	2	1.273
4	5	13.985	707.269	616.236	257.112	$1,3$	4	2	1.272
4	10	12.587	691.202	616.236	251.723	$1,3$	4	2	1.271
$5,6$	1	17.927	803.672	669.726	267.890	$1,3$	$2,5$	4	1.305
$5,6$	3	16.355	696.557	580.575	249.927	$1,3$	$2,5$	4	1.262
$5,6$	5	16.355	675.134	589.490	267.890	$1,4$	$2,5$	3	1.260
$5,6$	10	15.322	675.134	589.490	267.890	$1,4$	$3,5$	2	1.260

Table 10: Optimal solutions for three products with discrete tank sizes corresponding to the results of Table 9.

decisions s_p^M do not depend on the scenarios. We compare the stochastic solution with different deterministic approaches as follows. Treating each of the three scenarios as an independent deterministic optimization model may lead to different optimal tank sizes. Taking the expected tank sizes of those solutions and solving the corresponding non-linear lot-sizing problem with fixed tank sizes are shown in the rows where the second column reads 'exp-' for each of the three demand scenarios ('low', 'normal', 'high'). Another approach could be to use the maximum tank sizes instead of the expected tank sizes - those results are shown in the rows where the second column reads 'max-'.

Due to the nature of the stochastic approach, the optimal cost per ton of the stochastic solution cannot be higher than the expected cost per ton of the two approaches described above (for any given number of event points). We interpret this improvement of the stochastic approach as the value of the stochastic solution. For our data, the gains of the stochastic approach over the 'expected tank size' approach are 0.70%, 0.0258% and 0.182% and over the 'maximum tank size' approach are 0.069%, 0.069% and 0.075% for $N = 4, 5, 6$. These cost improvements are marginal. However, one has to take into account that only three scenarios for a three product case are discussed, where each scenario has an equal probability and the scenarios have very similar demands. Nevertheless, the computational results confirm the validity

N	case	s_1^M	s_2^M	s_3^M	T_1	T_2	T_3	T	c^{PT}	GAP	CPU
4	stochastic	691.105	619.115	253.294	12.510	11.367	9.658		1.252	0.00%	1:03:31
	exp-low							12.614	1.386	0.00%	0:00:03
4	exp-normal	683.983	621.149	253.654				11.370	1.269	0.00%	0:00:01
	exp-high							7.390	1.128	0.00%	0:00:01
	max-low							12.915	1.390	0.00%	0:00:02
4	max-normal	693.188	624.981	256.340				12.162	1.271	0.00%	0:00:01
	max-high							10.321	1.097	0.00%	0:00:02
5	stochastic	691.105	619.115	253.294	12.510	11.367	9.658		1.252	5.26%	‡
	exp-low							12.614	1.386	0.00%	0:00:04
5	exp-normal	683.983	621.149	253.654				11.370	1.269	0.00%	0:00:04
	exp-high							10.414	1.102	0.00%	0:00:04
	max-low							14.275	1.390	0.00%	0:00:06
5	max-normal	693.188	624.981	256.340				12.162	1.271	0.00%	0:00:05
	max-high							10.321	1.097	0.00%	0:00:05
6	stochastic	685.842	591.506	274.022	18.825	17.177	14.504		1.240	17.72%	‡
	exp-low							18.982	1.374	0.00%	0:00:11
6	exp-normal	680.312	594.628	274.523				17.232	1.258	0.00%	0:00:09
	exp-high							13.151	1.096	0.00%	0:00:12
	max-low							19.822	1.378	0.00%	0:00:12
6	max-normal	688.622	595.669	278.345				18.314	1.260	0.00%	0:00:16
	max-high							15.540	1.086	0.00%	0:00:11

‡ Time limit of 5h was reached.

Table 11: Computational results for stochastic demand with three products and three scenarios computed with LINDOGlobal. The results are compared to different deterministic cases.

of the stochastic approach.

8. Conclusion

We introduce a mixed-integer nonlinear programming formulation for a tank design problem, determining the optimal cycle time and the optimal campaign size. A continuous-time model is presented minimizing the cost per ton produced. Several properties of the model are discussed. In particular, the fact that the objective function value is a decreasing function in the number of event points is an important property of the model as it helps finding initial solutions and implies a natural way to stop the search for better solutions. Additional constraints in the model are presented to enhance computational efficiency and four model extensions are considered.

The computational tests show that nonlinear MINLP solver can provide good solutions while the two tested global solvers have difficulties proving global optimality. This suggests that the bounding in the global solvers can be improved by better exploiting the problem structure. The feasibility of the proposed model is demonstrated for examples with a small number of products.

As an important practical result our stochastic programming approach shows that the optimal tank-sizes do not vary significantly (only up to 3 or 5%) when the demand deviates between 10 and 20 % from the nominal demand.

Future research has to focus on the development of a theory for finding the optimal number of event points. This is in general a challenging task for continuous-time formulations. Furthermore, we plan to develop specialized global optimization solver tailored to the structure of the problem at hand.

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A. Indices and Sets

All indices, sets and dimensions used in the model are summarized in Table 12.

Set	Dim.	Description
$n \in \mathcal{N}$	N	Event points or campaigns
$p \in \mathcal{P}$	P	Products
$r \in \mathcal{R}$	R	Different reactors of the plant. This is only considered in the generalized model
$s \in \mathcal{S}$	S	Demand scenarios
$\tau \in \mathcal{T}_p$	$\lvert\mathcal{T}_p\rvert$	Different tanks for product p

Table 12: Indices, sets and dimensions of the model

B. Variables

The variables used in the model are given in Table 13. The units are shown in brackets "[]" in the second column. The domain of the variables is stated in the third column, where $\mathbf{R}_+$ are the non-negative real numbers, including 0 and $\{0, 1\}$ represents the binary domain. The index s (r) for a variables indicates that this variable depends on scenario s (reactor r).

C. Input Data

All input data are summarized in Table 14. Recognize that not all data have to be given explicitly. For instance, the minimal duration time of a campaign, D_p^-, might be given indirectly by the campaign setup-times, the inventory level and the demand rate. An additional index τ means that this data are with respect to a specific tank $\tau \in \mathcal{T}_p$. Similarly, the index s implies that the data correspond to scenario $s \in \mathcal{S}$.

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Var.	**Unit**	**Domain**	**Description**
c^{C}	[$]	$\mathbf{R}_+$	Campaign setup costs
c^{I}	[$]	$\mathbf{R}_+$	Tank investment costs. Given over a horizon of H years
c_s^{OPT}	[$/ton]	$\mathbf{R}_+$	Operational cost per ton for scenario s
c^{P}	[$]	$\mathbf{R}_+$	Variable production costs. They are excluded from the model as they are fix per ton
c^{PT}	[$/ton]	$\mathbf{R}_+$	Total cost per ton
c^{S}	[$]	$\mathbf{R}_+$	Variable tank cost
c^{T}	[$]	$\mathbf{R}_+$	Total costs
d_n	[days]	$\mathbf{R}_+$	Duration of production of campaign n
d_{nr}^{+}	[days]	$\mathbf{R}_+$	Duration of production of campaign n at reactor r
d_{nr}^{-}	[days]	$\mathbf{R}_+$	Duration of transferred setup-times from event point n on reactor r
$d_{nr}^{\times}$	[days]	$\mathbf{R}_+$	Duration shortage for the minimum campaign length of campaign n on reactor r
δ_{pnr}	[-]	$\mathbf{R}_+$	Indicates if production of product p starts at the beginning of event point n at reactor r
$\delta_{p\tau}$	[-]	SOS-1	Tank-investment variable selecting tank purchased for product p
$\lambda_{\overline{p}pn}$	[-]	$\mathbf{R}_+$	Auxiliary variables representing the product $\omega_{\overline{p}n-1}\omega_{pn}$
ω_{pn}	[-]	$\{0,1\}$	Task-event variable selecting product p produced in campaign n
p_{pn}^{C}	[tons]	$\mathbf{R}_+$	Produced amount of product p in campaign n
p_{pn}^{R}	[tons/day]	$\mathbf{R}_+$	Production rate for product p in campaign n
p^{T}	[tons]	$\mathbf{R}_+$	Total production over the planning period
s_{pn}	[tons]	$\mathbf{R}_+$	Stock or inventory of the tank corresponding to product p at the beginning of event point n
s_{pn}^{H}	[-]	$\mathbf{R}_+$	Auxiliary variables representing $\frac{s_{pn+1}+s_{pn}}{2}$
s_p^{M}	[tons]	$\mathbf{R}_+$	Design tank size storing product p
T	[days]	$\mathbf{R}_+$	Cycle time or planning horizon
t_n	[days]	$\mathbf{R}_+$	Length of campaign n
t_n^{SC}	[days]	$\mathbf{R}_+$	Setup-time for campaign n
y_{pn}	[days]	$\mathbf{R}_+$	Auxiliary variables representing product $d_n\omega_{pn}$

Table 13: Variables of the model

Data	Unit	Description
C_p^0	[\$/ton$^{0.5}$]	Variable part of the cost for the tank investment cost
C_p^{C}	[\$]	Fixed setup cost per campaign of product p
C_p^{F}	[\$]	Fixed part of the cost for the tank investment cost
C_p^{P}	[\$/ton]	Variable production cost for product p
C_p^{S}	[\$/ton/day]	Variable inventory cost
H	[years]	Time horizon of investment cost for the tanks
C_p^-	[tons]	Lower limit on the production amount per campaign of product p
C_p^+	[tons]	Upper limit on the production amount per campaign of product p
D_p	[tons/year]	Demand of product p per year
D_p^-	[days]	Minimal duration of a campaign
D_p^+	[days]	Maximal duration of a campaign
L	[tons/day]	Total demand per day
L_p	[tons/day]	Demand of product p per day
$P_p^{\mathrm{R}-}$	[tons/day]	Lower limit on the production rate of product p
$P_p^{\mathrm{R}+}$	[tons/day]	Upper limit on the production rate of product p
Pr_s	[-]	Probability for scenario s
S_p^-	[tons]	Safety stock for product p. This is a lower bound on the tank inventory for product p
S_p^+	[tons]	Maximal tank capacity for product p. This is an upper bound on the tank inventory for product p as well as an upper bound on the tank size s_p^{M}
T_p^{S}	[days]	Setup-time for product p. The value is independent of the sequence
$T_{\overline{p}p}^{\mathrm{S}}$	[days]	Sequence-dependent setup-time for product p preceding the production of product $\overline{p}$

Table 14: Input data for the model

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