This item is the archived peer-reviewed author-version of:

Design of a chemical batch plant with parallel production lines : plant configuration and cost effectiveness

Reference:

Verbiest Floor, Cornelissens Trijntje, Springael Johan.- Design of a chemical batch plant with parallel production lines : plant configuration and cost effectiveness
Computers and chemical engineering - ISSN 0098-1354 - 99(2017), p. 21-30
Full text (Publisher's DOI): <https://doi.org/10.1016/J.COMPCHEMENG.2016.12.013>
To cite this reference: <https://hdl.handle.net/10067/1395460151162165141>

Design of a chemical batch plant with parallel production lines: plant configuration and cost effectiveness

Floor Verbiest^{a,*}, Trijntje Cornelissens^a, Johan Springael^a

^aANT/OR - Operations Research Group,
Department of Engineering Management,
University of Antwerp, Prinsstraat 13, 2000 Antwerp, Belgium

Abstract

We present a model for the design of multiproduct sequential batch plants extended with parallel production lines. This model is meant to support strategic capacity decisions and is formulated as a MILP model. First, we introduce the concept of parallel production lines as a new design option into existing plant design models. Then, we optimise the number of production lines, their design and the product assignment to the installed lines by minimising capital costs of the equipment. Furthermore, we extend the objective function with startup and contamination costs and study the influence of these costs on the chosen plant design options. We find the presence of parallel production lines beneficial as not all products have to share all equipment anymore. Moreover, we show that the incorporation of operating costs affects volume-wise asset utilisation per batch. An example to illustrate the applicability of our model is presented.

Keywords: chemical batch plant, plant design, parallel production lines

---

1. Introduction

1.1. Research context

Increasing pressure on supply chain performance forces production companies nowadays to take appropriate strategic decisions on plant design. We focus

---

*Corresponding author

Email address: floor.verbiest@uantwerpen.be (Floor Verbiest)

5 on such decisions for chemical batch plants in a flow shop environment in particular. Batch plants are typically equipped with tanks and reactors, in which all the input material is treated for a certain period of time and then passed on to the next operation (and equipment) ([Rippin, 1983](#)).

10 The design of such plants at a strategic decision level considers plant configuration (i.e. number, size and connectivity of equipment), the related batch sizes of the different manufactured products and the related production policy (e.g. campaign length, product-equipment dedication). This design depends on several strategic choices on production environment, mode of operation, design
15 options and the business objective.

The plant design problem has been studied extensively in the past. [Loonkar and Robinson \(1970\)](#) calculated the optimal equipment sizes for a single product batch plant with one production line. The objective of their nonlinear program
20 was to minimise capital investment via iteratively solved algebraic equations. By extending this model to batch plants producing different products, two major production environments are considered in literature: multiproduct plants, also denoted as flow shops, and multipurpose plants or job shops. Among the pioneering work on multiproduct plants, [Sparrow et al. \(1975\)](#) solved the design
25 problem extended with parallel equipment per processing stage, assuming single product campaign mode of operation, by both a branch-and-bound method and a heuristic approach. [Grossmann and Sargent \(1979\)](#) formulated this problem as a mixed-integer nonlinear programming problem (MINLP), which was later reformulated as a linear problem (MILP) by [Voudouris and Grossmann \(1992\)](#).
30 Other multiproduct design models were extended for semicontinuous- and intermediate storage equipment, but still consider a single production line ([Knopf et al., 1982](#); [Takamatsu et al., 1982](#); [Modi and Karimi, 1989](#)). A review on the design of multiproduct and multipurpose plants is presented by [Barbosa-Póvoa \(2007\)](#). The aim of all the aforementioned design problems is to minimise capital costs, however other costs have been included as well: e.g. the minimisation
35

of energy costs (Knopf et al., 1982) and of environmental impact (Dietz et al., 2006). Some articles consider profit maximisation and include, besides capital costs, also e.g. raw material and disposal (e.g. Corsano et al., 2007; Moreno and Montagna, 2007) and maintenance costs (Pistikopoulos et al., 1996; Goel et al., 2003).

Moreover, in order to better incorporate the operational use of a plant, the plant design models incorporated scheduling techniques. In these design and scheduling papers, the problems are classified into two categories according to process topology: sequential and network processes. In sequential processes, each batch is processed following a sequence of stages and the identity of the batch is preserved. In more complex network processes, batch mixing, splitting as well as material recycling occurs and material balances are needed to describe all the flows. Furthermore, two modes of operation can be distinguished: cyclic and non-cyclic. Cyclic models assume a campaign mode of operation, whereas in non-cyclic models production may occur at arbitrary points in time and in arbitrary sequences. For network processes, the design problem is solved incorporating both (non-cyclic) discrete-time and continuous-time formulations. Barbosa-Póvoa and Macchietto (1994) presented a discrete-time maximal State Task Network (STN) representation, based on the original STN formulation of Kondili et al. (1993). Barbosa-Póvoa and Pantelides (1997) and Pinto et al. (2005) developed a discrete-time model relying on the Resource Task Network (RTN) framework. Continuous-time models are reported by Xia and Macchietto (1997), Lin and Floudas (2001) and Seid and Majozi (2013) based on the STN formulation and by Castro et al. (2005) based on the RTN representation. All these models optimise multipurpose plants with complex processes that are well suited for a network representation. We refer to recent review papers on short-term batch scheduling for a more complete overview (Floudas and Lin, 2004; Méndez et al., 2006; Harjunkski et al., 2014). Alternatively, literature on plant design models for sequential processes consider mostly a cyclic mode of operation. Birewar and Grossmann (1989, 1990) introduced multiple product

campaigns as opposed to the single product campaigns. More recently, the combination of designing and cyclic scheduling via multiple product campaigns has been studied e.g. by [Corsano et al. \(2007\)](#) using a heuristic solution method and
70 by [Fumero et al. \(2013\)](#) solving a MILP model extended for parallel machines in each stage of the production process.

The above literature overview illustrates the several strategic choices that affect the design: on production environment (the production of single or multiple
75 products, in multiproduct or multipurpose plants, etc.), on mode of operation (cyclic or non-cyclic), on the business objective (cost minimisation and profit maximisation) and on the design options allowed. It is on this last strategic choice that we will focus in this paper.

80 In the aforementioned literature on chemical batch plant design, there are several design options reported: the introduction of parallel equipment per stage and/or intermediate storage between stages. These options aim at eliminating or reducing capacity issues which slow down the entire process. Indeed, these design options lead to shorter cycle times, hence more batches in smaller and
85 thus cheaper equipment. In practice however, we observe another design option that is frequently used in chemical plants, namely the installation of parallel production lines. These parallel lines are installed on one production site and operate independently but simultaneously with each other. The lines have the same processing steps and hence products may be produced on multiple lines.
90 As total production volume is now divided over these lines, products can be dedicated to lines, which may reduce the required size and/or number of the capital intensive stages.

We found the presence of comparable parallel lines in batch plants in several
95 types of short-term scheduling articles. However, all these articles assume a given design. On the one hand, parallel lines are referred to in scheduling on single-stage batch plants with nonidentical equipment that work independently.

A MILP model was presented for the scheduling of single-stage parallel-line multiproduct batch plants based on batch precedence (Cerdá et al., 1997), and time-slots (Chen et al., 2002), which was extended with resource constraints and raw material supplies by Lamba and Karimi (2002). This type of problems are also referred to as parallel flowshop models (Gooding et al., 1994). On the other hand, in literature on short-term scheduling in multistage, sequential batch plants some semi-parallel lines occur. In these articles, there is limited connectivity between some equipment, but the lines are not entirely separated nor do they work independently. Pinto and Grossmann (1995) developed a MILP model with time-slots for the scheduling of multistage batch plants with parallel equipment. The model is based on parallel time coordinates for units and tasks. Méndez et al. (2001) proposed a mathematical model for the resource-constrained short-term scheduling problem. They considered a sequential batch plant with multiple stages and several units working in parallel, where assignment and sequencing decisions are handled independently. Recently, however, Hill et al. (2016) proposed a scheduling heuristic for realistic production planning in a multiproduct, multistage blending plant with parallel production lines as defined previously.

1.2. Contributions

In this paper, a MILP model is proposed for determining the design of sequential multiproduct batch plants, operating in cyclic mode. However, in addition to existing design models, the strategic decision of installing parallel lines and, if so, how many is explicitly taken into account.

Next, we solve this design problem not only for the minimisation of capital costs of the batch equipment, but we include additional cost components such as setup costs and product-batch related operating costs. We assume in this paper that the business objective is to optimise cost effectiveness.

Regarding the setup costs, we distinguish two components: a startup and

contamination cost. The fixed startup cost is incurred for every equipment unit, every time a series of batches of the same product starts and represents the cost of setting the equipment parameters to the required level (such as temperature and pressure), preparing the inflow of ingredients, performing quality tests, etc. When parallel production lines are installed, a decrease in the total startup cost can be expected if there is a reduction in number of equipment used per product. The contamination cost, on the other hand, depends on the combination of products produced on the same equipment units. In practice, products with similar characteristics are often grouped into product families. As products from different families often generate contamination among each other, it is preferred to produce them not on the same line. Consequently, if production lines are installed and dedicated to certain products/product families, high contamination costs can be avoided.

Finally, we consider an operating cost that accounts for labour, use of utilities, etc. per batch of every product. Because of the variable character of this cost component, i.e. dependent on the number of batches, production of the demand in the least number of batches is favoured. If this operating cost does not influence the design choices, a consequence of minimising this operating cost is an increase in volume-wise asset utilisation per batch. Time-wise asset utilisation, on the other hand, will be lower, and thus idle time will occur. However, this phenomenon can provide a welcome buffer for small unforeseen events.

2. Problem formulation and assumptions

The chemical batch plant considered in this paper is a multiproduct plant designed for a multistage process. Production is represented by a flow of batches and material balances can be omitted, so a sequential representation is chosen.

We consider P products i that are to be produced over J stages j , where every stage performs an operation. The demand for every product (Q_i) and the

total production horizon (H) are known upfront, as well as the characteristic size factors (S_{ij}) and the fixed batch processing times (τ_{ij}). The size factors correspond to the characteristic size of equipment needed at stage j to produce unit mass of product i . The batch processing times are the durations of the operations in stage j for product i and are independent of the product batch size. Further assumptions are:

1. Production process/recipes are known upfront;
2. Unlimited access to raw materials;
3. Only batch equipment is explicitly considered;
4. Zero-wait policy between the batch stages;
5. Overlapping mode of operation;
6. At most N identical parallel equipment per stage (n_j), operating out-of-phase (see Fig. 1, stage 1);
7. Cycle time of product i is the longest stage cycle time over all stages: $\max_{j=1,\dots,J} \tau_{ij}/n_j$ (see Fig. 1);
8. Deterministic demand and process parameters;
9. Discrete set of S equipment sizes v_s for all stages j to choose from;
10. Single product campaign mode of operation (see Fig. 1) and no intermediate due dates.

This last assumption implies that no explicit sequencing nor specified start and end times are needed (Applequist et al., 1997). Although this is a simplification of reality, it does not harm the motivation and importance of installing parallel production lines. More explicit scheduling should be addressed in future work.

Figure 1: Illustration of single product campaigns, parallel equipment operating out-of-phase in stage 1 and product cycle times for a single production line (Adapted from Biegler et al., 1997)

Our first contribution involves the introduction of parallel lines as a decision variable, where we assume that there are at most L lines l to install, with on every line J stages j . Since all products i are allowed on all lines l , production of the products can be split over lines. And thus, given the assumptions, the aim is to determine:

- The optimal number of lines l to install;
- Per stage of every installed line: the optimal number n and size s of equipment;
- The assignment of products to the installed lines, which includes:
  - the amount produced of every product i on every line l (q_{li});
  - the number of batches, and the corresponding batch sizes, of every product i on every line l (n_{li});
  - the time spent on every product i on every line l (θ_{li}).

3. Mathematical model

In this section, we present a MILP model that includes design, horizon and demand constraints and the objective function to be minimised. This objective consists of the different cost components as also described in Section 1.2. The nomenclature used in this model is provided in Appendix A.

3.1. Constraints

200 *Production line design constraints:*

In order to determine the existence of lines, and more precisely of stages and parallel equipment per stage, the binary z_{ljn} is defined:

$$z_{ljn} = \begin{cases} 1 & \text{if unit } n \text{ of stage } j \text{ of line } l \text{ exists} \\ 0 & \text{otherwise} \end{cases}$$

This variable explicitly accounts for the existence of equipment units, with $\sum_{n=1}^N z_{ljn} \leq N \quad \forall l, j$. The resulting constraints are:

$$\sum_{n=1}^N z_{lj'n} \leq N \sum_{n=1}^N z_{ljn} \quad \forall l, j, j' \quad (1)$$

$$z_{ljn} \geq z_{lj(n+1)} \quad \forall l, j, n \text{ with } n < N \quad (2)$$

Eq.(1) states that if a stage of a line does not exist, the remaining stages of the same line are also non existent. Eq.(2) indicates that equipment $n + 1$ of stage j of line l will only be installed if equipment n already exists.

Furthermore, the related assignment of products to the installed lines is indicated with:

$$t_{li} = \begin{cases} 1 & \text{if product } i \text{ is produced on line } l \\ 0 & \text{otherwise} \end{cases}$$

so that the following constraints apply:

$$t_{li} \leq \sum_{n=1}^N z_{ljn} \quad \forall l, j, i \quad (3)$$

$$\sum_{l=1}^L t_{li} \geq 1 \quad \forall i \quad (4)$$

205 Eq.(3) means that no product can be assigned to a line that does not exist and Eq.(4) indicates that every product is produced on at least 1 line.

Equipment design constraints:

To determine the size of the equipment, we introduce the binary variable:

$$u_{ljs} = \begin{cases} 1 & \text{if equipment of stage } j \text{ of line } l \text{ has size } s \\ 0 & \text{otherwise} \end{cases}$$

which is used in the following constraints:

$$\sum_{n=1}^N z_{ljn} \leq N \sum_{s=1}^S u_{ljs} \quad \forall l, j \quad (5)$$

$$\sum_{n=1}^N z_{ljn} \geq \sum_{s=1}^S u_{ljs} \quad \forall l, j \quad (6)$$

$$\sum_{s=1}^S u_{ljs} \leq 1 \quad \forall l, j \quad (7)$$

$$n_{li} \geq \sum_{s=1}^S \frac{q_{li} S_{ij}}{v_s} u_{ljs} \quad \forall l, j, i \quad (8)$$

Eq.(5)-(6) define the relation between the existence of a stage and the choice of the equipment size for that stage. Eq.(5) forces the choice of a size if equipment is installed at stage j of line l . Eq.(6), on the other hand, states that if no equipment is installed at stage j of line l , then no size is chosen. Overall, for every stage j at most 1 size s is chosen (Eq.(7)). Furthermore, for every stage j of line l the capacity of the equipment v_s should be large enough to hold a batch of every product i , multiplied by its size factor S_{ij} . Incorporating the discrete set of sizes gives Eq.(8).

Taking into account the bilinear product of a continuous and binary variable $Z_{ljis} = q_{li} u_{ljs}$, we rewrite Eq.(8):

$$n_{li} \geq \sum_{s=1}^S \frac{S_{ij}}{v_s} Z_{ljis} \quad \forall l, j, i \quad (9)$$

and add the following linearisation constraints:

$$Z_{ljis} \leq Q_i u_{ljs} \quad \forall l, j, i, s \quad (10)$$

$$Z_{ljis} \leq q_{li} \quad \forall l, j, i, s \quad (11)$$

$$Z_{ljis} \geq q_{li} - Q_i(1 - u_{ljs}) \quad \forall l, j, i, s \quad (12)$$

$$Z_{ljis} \geq 0 \quad (13)$$

Horizon constraints:

$$\sum_{n=1}^N z_{ljn} T_{lji} = n_{li} \tau_{ij} \quad \forall l, j, i \quad (14)$$

$$\theta_{li} \geq T_{lji} \quad \forall l, j, i \quad (15)$$

$$\sum_{i=1}^P \theta_{li} \leq H \quad \forall l \quad (16)$$

Total time spent on every product i on stage j of line l (T_{lji}) corresponds to the time spent per batch (stage cycle time) multiplied by the number of batches (Eq.(14)). Indeed, as explained in Section 2, and illustrated on Figure 1, parallel equipment per stage operate out-of-phase and influence the time necessary to produce a batch. Total time spent on every product i on a line l (θ_{li}) corresponds to the longest time spent on a stage of that line (Eq.(15)). Furthermore, total production time per line should not exceed the production horizon H (Eq.(16)).

225

We replace the nonlinear Eq.(14) by a linear equivalent via the newly introduced continuous variable $X_{ljin} = z_{ljn} T_{lji}$:

$$\sum_{n=1}^N X_{ljin} = n_{li} \tau_{ij} \quad \forall l, j, i \quad (17)$$

and add the following linearisation constraints:

$$X_{ljin} \leq H z_{ljn} \quad \forall l, j, i, n \quad (18)$$

$$X_{ljin} \leq T_{lji} \quad \forall l, j, i, n \quad (19)$$

$$X_{ljin} \geq T_{lji} - H(1 - z_{ljn}) \quad \forall l, j, i, n \quad (20)$$

$$X_{ljin} \geq 0 \quad (21)$$

Demand constraint

$$\sum_{l=1}^L q_{li} = Q_i \quad \forall i \quad (22)$$

The production of product i split over multiple lines l should sum up to the demand (Eq.(22)).

Boundaries

$$q_{li} \leq Q_i t_{li} \quad \forall l, i \quad (23)$$

$$n_{li} \leq M_i t_{li} \quad \forall l, i \quad (24)$$

$$T_{lji} \leq H t_{li} \quad \forall l, j, i \quad (25)$$

$$\theta_{li} \leq H t_{li} \quad \forall l, i \quad (26)$$

$$\epsilon t_{li} \leq q_{li} \quad \forall l, i \quad (27)$$

Eq.(23)-(26) pose an upper bound on the variables. If product i is not produced on line l ($t_{li} = 0$), then no amount of (q_{li}), no batches of (n_{li}) and no time on (T_{lji} and θ_{li}) product i is produced or spent. We have included M_i as an upper bound on the number of batches for every product i , which is formulated as $(Q_i S_{ij}^{max})/v_0$. Indeed, the maximum number of batches occur when the total amount (Q_i) has to be produced in the smallest available tank (v_0), taking into account the largest size factor S_{ij}^{max} per product. Eq.(27) is to make sure that if no amount is produced of product i on line l , then this product is not produced at all on that line, where ϵ is a very small positive number.

3.2. Objective function

As stated, the objective function consists of several cost components which are discussed below.

3.2.1. Minimisation of capital costs

At first, we minimise the capital costs:

$$\sum_{l=1}^L \sum_{j=1}^J \sum_{s=1}^S \sum_{n=1}^N c_{js} z_{ljn} u_{ljs}$$

with $c_{js} = \alpha_j v_s^{\beta_j}$ and α_j, β_j the stage dependent cost coefficients. In order to correctly sum up this one time capital expenditure with the other cost components (Jelen et al., 1983), we assume that the conversion to a uniform cost per horizon is already done. The product of the binaries z_{ljn} and u_{ljs} is replaced with Y_{ljsn} and the constraints:

$$Y_{ljsn} \geq u_{ljs} + z_{ljn} - 1 \quad \forall l, j, s, n \quad (28)$$

$$Y_{ljsn} \in \{0, 1\} \quad (29)$$

3.2.2. Minimisation of setup costs

We implement a twofold setup cost, i.e. a startup and contamination cost,
245 which are both independent of the volume or number of batches.

Startup costs. The preparation of the equipment units at the start of every series of batches of product i is modelled as follows:

$$\sum_{i=1}^P \sum_{l=1}^L \sum_{j=1}^J \sum_{n=1}^N Cstart_i z_{ljn} t_{li}$$

where $Cstart_i$ is a line and stage independent startup cost. If t_{li} equals one, all the equipment units of line l , given by $\sum_{j=1}^J \sum_{n=1}^N z_{ljn}$, have to be configured for producing product i .

This nonlinear cost component is linearised by introducing the binary variable $V_{ljin} = t_{li} z_{ljn}$ and:

$$V_{ljin} \geq z_{ljn} + t_{li} - 1 \quad \forall l, j, i, n \quad (30)$$

$$V_{ljin} \in \{0, 1\} \quad (31)$$

Contamination costs. As stated, the contamination cost represents a penalisation for producing products from different product families on the same equipment/line. As in this paper, we do not determine the exact sequence of products, we assume a fixed cost C_{cont} that occurs when changing from one product family to another for all equipment units on a production line. We introduce the binary variable b_{fl} that indicates if product family f is produced on line l . This is calculated via the constraint:

$$b_{fl} \geq d_{if} t_{li} \quad \forall l, f, i \quad (32)$$

with d_{if} the boolean matrix indicating if product i belongs to family f , which is known upfront. This results in the following contamination cost:

$$\sum_{l=1}^L \sum_{j=1}^J \sum_{f=1}^F \sum_{n=1}^N C_{cont} b_{fl} z_{ljn}$$

By introducing $U_{ljfn} = b_{fl} z_{ljn}$ and:

$$U_{ljfn} \geq z_{ljn} + b_{fl} - 1 \quad \forall l, j, f, n \quad (33)$$

$$U_{ljfn} \in \{0, 1\} \quad (34)$$

we obtain a linearised contamination cost:

$$\sum_{l=1}^L \sum_{j=1}^J \sum_{f=1}^F \sum_{n=1}^N C_{cont} U_{ljfn}$$

However, this formulation also generates a contamination cost when there is only one product family on a line. To avoid this, we include a correction via the binary g_l .

$$\sum_{l=1}^L \sum_{j=1}^J \sum_{f=1}^F \sum_{n=1}^N C_{cont} U_{ljfn} g_l$$

$$\sum_{f=1}^F b_{fl} \geq 2 - M(1 - g_l) \quad \forall l \quad (35)$$

$$\sum_{f=1}^F b_{fl} - 1 \leq M g_l \quad \forall l \quad (36)$$

These constraints force g_l to zero if there is no or 1 product family on the equipment, with M a very large positive number. Otherwise, g_l is 1 and there is a contamination cost for all product families and all equipment units on that line. The nonlinearity is again tackled via $H_{ljfn} = g_l U_{ljfn}$ and:

$$H_{ljfn} \geq U_{ljfn} + g_l - 1 \quad \forall l, j, f, n \quad (37)$$

$$H_{ljfn} \in \{0, 1\} \quad (38)$$

The resulting contamination cost is now:

$$\sum_{l=1}^L \sum_{j=1}^J \sum_{f=1}^F \sum_{n=1}^N C_{cont} H_{ljfn}$$

Eventually the extended MILP is:

$$\min \left[\sum_{l=1}^L \sum_{j=1}^J \sum_{s=1}^S \sum_{n=1}^N c_{js} Y_{ljfn} + \sum_{i=1}^P \sum_{l=1}^L \sum_{j=1}^J \sum_{n=1}^N C_{start_i} V_{ljin} + \sum_{l=1}^L \sum_{j=1}^J \sum_{f=1}^F \sum_{n=1}^N C_{cont} H_{ljfn} \right]$$

250 s.t. (1)-(7), (9)-(13) and (15)-(38).

3.2.3. Minimisation of operating costs

Finally, to take into account the variable production cost, we add the following operating cost to the objective function:

$$\sum_{l=1}^L \sum_{i=1}^P C_{operat_i} n_{li}$$

Minimising this operating cost, within the bounds of the installed equipment, corresponds to minimising the number of batches, or equivalently maximising the batch sizes. Fewer batches imply lower operating costs and, as a result, also a higher volume-wise capacity utilisation per batch. This volume-wise utilisation was calculated as $(B_{li} S_{ij})/v_s$ for every product on every stage, with $B_{li} = q_{li}/n_{li}$. As fewer batches are needed to produce total demand of every product, idle time will occur. Hence, time-wise asset utilisation will be lower but, as stated in Section 1.2, this can be seen as a positive side-effect.

260 4. Illustrative example

4.1. Process description

We illustrate the implementation of parallel production lines as a strategic design option with the following example. The aim is to design a chemical batch plant that needs to produce 8 products with a given demand within a
265 given production horizon. As stated before, production is done in single product campaign mode of operation. The plant surface area allows for the installation of at most 3 lines over which total production can be divided. The production process for all products consists of 3 operations, performed in 3 stages. All input data is given in Table 1. As can be seen from this table, the operation in stage
270 3 is the longest and has also the most expensive equipment (given by α and β), so stage 3 can be considered as the bottleneck of the entire production process.

Table 1: Process and demand data

Design options:								
Parallel lines: min 1 - max 3								
Parallel equipment per stage: min 1 - max 3								
Product demand Q_i (x 1,000 in kg)								
	prod 1	prod 2	prod 3	prod 4	prod 5	prod 6	prod 7	prod 8
	500	250	150	300	400	420	275	175
Processing time τ_{ij} (in h)								
stage 1	3.2	3.1	2.0	2.5	1.9	2.8	1.8	3.5
stage 2	2.0	1.6	2.3	3.0	2.2	3.2	4.0	2.8
stage 3	8.6	11.5	7.0	8.3	12.3	9.4	10.6	6.8
Size factor S_{ij} (in l/kg)								
stage 1	1.3	1.0	1.2	1.1	1.3	1.4	1.6	1.8
stage 2	1.4	1.5	1.1	0.9	1.0	1.2	1.5	1.3
stage 3	1.0	1.6	1.3	1.7	1.0	1.6	1.2	1.1
Horizon H (in h) = 6,500								
Set S of discrete sizes v_s (in l) = {400, 600, 800, 1,000, 1,200, 1,400, 1,600, 1,800, 2,000, 2,200}								
Cost coefficients $\alpha_j = \{150, 200, 450\}$ and $\beta_j = \{0.25, 0.45, 0.70\}$								

This example is analysed for 3 objective functions: the minimisation of (1) only capital costs; (2) of capital and startup costs and (3) of capital, startup and contamination costs (see additional data in Table 2). For every objective
275 function, we solve and compare two cases with case 1 being the design of a

plant with 1 production line and case 2 the design when multiple production lines are allowed. Furthermore, we analyse and optimise operating costs within the chosen design.

280 All numerical results are obtained using the Gurobi Optimizer 6.5 (Gurobi, 2016) on an Intel(R) Core i7 - 5600U CPU, 2.6 GHz computer and a visual overview is given in Appendix B.

Table 2: Additional data for objective functions (2) and (3): including setup costs

Startup costs $Cstart_i$							
prod 1	prod 2	prod 3	prod 4	prod 5	prod 6	prod 7	prod 8
2,750	1,800	2,000	3,150	3,200	2,500	3,800	4,000
Contamination cost between product families $Ccont = 7,000$							
Product families: $P_{f1} = \{1, 3, 4, 5, 8\}$ and $P_{f2} = \{2, 6, 7\}$							

4.2. Results

4.2.1. Minimisation of capital costs

285 The solution of the example when minimising only capital costs is shown in Table 3. The left panel (case 1) gives the optimal solution when there is only one production line. The right panel (case 2) shows the optimal design for a plant when parallel production lines are allowed.

290 As can be seen from Table 3, it is optimal to install 2 parallel lines over which production can be divided. When we look into more detail to the capital costs, we notice a decrease in the costs of every stage: 2,055 vs 2,030 for stage 1, 12,769 vs 11,666 for stage 2 and 236,166 vs 235,339 for stage 3. Of course, this difference is rather small and in case of less dominant costs of stage 3 equipment,
295 it may be optimal to install only 1 line. The lower panel of the table gives the optimal distribution of production over the 2 lines. For this example, production of product 6 and 7 is split over 2 lines while the remaining products (1, 2, 3, 4, 5 and 8) are manufactured on one line each, with products 2, 3, 4 and 5 on line 1 and products 1 and 8 on line 2.

Table 3: Solution at minimum capital cost: design of plant with one line (case 1) and multiple lines (case 2)

Case 1: one production line		Case 2: multiple production lines			
Capital costs = 250,990		Capital costs = 249,035			
	size (numb)	line 1 size (numb)	line 2 size (numb)	line 3 size (numb)	
stage 1	2,200 (2)	stage 1 2,200 (1)	2,000 (1)	0	
stage 2	2,200 (2)	stage 2 1,800 (1)	1,800 (1)	0	
stage 3	1,600 (3)	stage 3 1,800 (2)	1,200 (1)	0	

Product assignment for case 2: q_{li} (x 1,000 in kg)								
	prod 1	prod 2	prod 3	prod 4	prod 5	prod 6	prod 7	prod 8
line 1	0	250	150	300	400	416	108	0
line 2	500	0	0	0	0	4	167	175
line 3	0	0	0	0	0	0	0	0

Problem size case 1: 826 var.(90 bin.var.); 2,236 const., solved in 0.06 s

Problem size case 2: 1,491 var.(411 bin.var.); 3,607 const., solved in 138.4 s

300 4.2.2. Minimisation of capital and startup costs

Table 4 gives the optimal solution for the two cases when startup costs are included. For case 1, as a result of the minimisation of the startup costs, the number of equipment decreased in comparison with the results in Table 3 (5 instead of 7 tanks). This is at the expense of larger bottleneck tanks which
305 outweigh the decrease in number of equipment units, leading to an increase in capital costs. For case 2, it seems optimal to install an extra line, 3 lines in total, so that only 1 line for every product is used and each stage has 1 equipment unit. As a consequence, as not all products have to share all equipment, total startup costs are lower than is the case for a single production line. When we
310 look again at the cost structure of the 2 cases, we notice for case 2 an increase in capital costs of stage 1 and 2 compared to case 1 (21,132 vs 7,412), as there are 6 equipment units in stage 1 and 2 (case 2) instead of 2 (case 1). However, there is a decrease in costs of stage 3 for the case with parallel lines (235,907 vs 256,463). It even outweighs the increase of stage 1 and 2 so that total capital
315 costs are, in this example, again lower with parallel lines than without.

Table 4: Solution at minimum capital and startup cost: design of plant with one line (case 1) and multiple lines (case 2)

Case 1: one production line			Case 2: multiple production lines					
Total costs = 379,875 (Capital: 263,875 + Startup: 116,000)			Total costs = 326,639 (Capital: 257,039 + Startup: 69,600)					
	size (numb)		line 1 size (numb)	line 2 size (numb)	line 3 size (numb)			
stage 1	2,200 (1)		stage 1 2,200 (1)	2,200 (1)	2,200 (1)			
stage 2	2,200 (1)		stage 2 1,800 (1)	1,800 (1)	2,200 (1)			
stage 3	1,800 (3)		stage 3 1,800 (1)	1,400 (1)	1,600 (1)			
Product assignment for case 2: q_{li} (x 1,000 in kg)								
	prod 1	prod 2	prod 3	prod 4	prod 5	prod 6	prod 7	prod 8
line 1	0	0	0	0	400	420	0	0
line 2	0	0	0	300	0	0	275	175
line 3	500	250	150	0	0	0	0	0

Problem size case 1: 827 var.(90 bin.var.); 2,237 const., solved in 0.08 s

Problem size case 2: 1,707 var.(627 bin.var.); 3,823 const., solved in 565.5 s

Sensitivity analysis of startup costs: As shown in Table 4, the incorporation of startup costs into the objective function can have an impact on the design decisions. In the following part, we investigate the impact of startup costs on the optimal design, or equivalently on the capital costs. We assumed that the input data shown in Table 1 remained constant.

The cost functions are plotted for a plant consisting of 2 and 3 parallel lines (see Fig. 2). We start with no startup costs and then gradually increase these costs with 150 for 15 iterations. As we are particularly interested in the impact of the total startup costs on design, we assumed startup costs the same for all products. The first solution corresponds to the situation when there are only capital costs (249,035 for 2 lines vs 253,584 for 3 lines). For the first iterations, startup costs are slightly higher for the solution with 2 parallel lines as one of the lines has 4 equipment units, whereas for the solution with 3 parallel lines all lines have only one unit per stage. However, in total, the option with 2 parallel lines is less expensive. The small cracks in the curves in the following iterations represent redistributions of products over the lines and corresponding (small)

Figure 2: Sensitivity analysis of startup costs

design changes. However, at iteration 9, there is a jump in capital and startup costs for the design with 3 parallel lines. From here on, it is better to install
335 larger tanks (capital costs increase from 253,584 to 257,039), in order to have only once per product a startup cost and thus, to use 3 equipment units (1 line) per product. At iteration 10, the two design options intersect and have the same total costs. From iteration 11, it is beneficial to install the extra production line, and to increase the capital costs to 257,039, so that startup costs are reduced
340 (36,000 instead of the expected 43,500) and every product uses 1 line, with 1 equipment unit on every stage. After that, no change in design occurred and we have the solution presented in Table 4, case 2.

4.2.3. Minimisation of capital, startup and contamination costs

Table 5 gives the results when contamination costs are included as a penal-
345 isation for producing contaminating product families on the same line. As can be seen, the number and sizes of equipment for case 1 are identical to the ones found in Table 4, hence capital and startup costs remained the same. A contamination cost incurred for every product family, since they all use the same equipment. After all, when there is only one production line, dedicating equip-

ment to products (product families) is not possible and additional treatments
have to be performed either way. In case 2, we can avoid these contamination
costs, which allows us to conclude that parallel production lines are beneficial
when product families can be separated. From the product assignments shown
in the lower panel of Table 5, we notice a rearrangement of the products over
the lines so that product families are produced together. This rearrangement
results in an increase in capital and startup costs. Eventually, this combination
of products on lines is the production policy that has to be adopted.

Table 5: Solution at minimum capital, startup and contamination cost: design of plant with
one line (case 1) and multiple lines (case 2)

Case 1: one production line		Case 2: multiple production lines			
Total costs = 449,875 (Capital: 263,875 + Startup: 116,000 + Cont: 70,000)		Total costs = 360,326 (Capital: 282,626 + Startup: 77,700 + Cont: 0)			
	size (numb)	line 1 size (numb)	line 2 size (numb)	line 3 size (numb)	
stage 1	2,200 (1)	stage 1 2,000 (1)	1,200 (1)	1,400 (1)	
stage 2	2,200 (1)	stage 2 2,200 (1)	1,200 (1)	1,000 (1)	
stage 3	1,800 (3)	stage 3 1,600 (1)	1,200 (2)	1,000 (1)	

Product assignment for case 2: q_{li} (x 1,000 in kg)								
	prod 1	prod 2	prod 3	prod 4	prod 5	prod 6	prod 7	prod 8
line 1	500	0	150	300	0	0	0	0
line 2	0	250	0	0	0	420	275	0
line 3	0	0	0	0	400	0	0	175

Problem size case 1: 835 var.(90 bin.var.); 2,213 const., solved in 0.62 s

Problem size case 2: 1,824 var.(744 bin.var.); 3,985 const., solved in 720.5 s

4.2.4. Minimisation of operating costs

In the third and last continuation of our example, we include the operating
cost per batch and study the influence of these costs on the volume-wise asset
efficiency. The results for case 2 of Table 5 (multiple lines) with operating costs
are shown in Table 6. The effect of including operating costs is similar for all
cases. Indeed, it was found that, without operating costs, for every line produc-
tion is spread over the total horizon and there is at least one product for which
there is still a range of batch sizes allowed within the installed equipment, so for

these products no stage is used for a 100 %. When including the operating costs, the number of batches of these products are forced to the minimum. Hence, the batch sizes are maximised, leading to a 100 % utilisation for every product for at least one stage. Or in other words, when these operating costs are included, the upper volume-wise utilisation percentage of the range is considered. For the remaining products, the results indicate that, even without operating cost, the products are produced in the minimum number of batches, or equivalently, in the maximum batch sizes. Finally, the reduction in total number of batches produced involves a shorter total production time for every line (i.e. before the end of the production horizon of 6,500 h).

Table 6: Volume-wise equipment utilisation per line in % - case 2 of Table 5

	<i>Line 1</i>			<i>Line 2</i>			<i>Line 3</i>	
	prod 1	prod 3	prod 4	prod 2	prod 6	prod 7	prod 5	prod 8
stage 1	93.1→ 100	73.8	51.8	62.2→62.5	87.5	100	92.2→92.9	98.9
stage 2	91.2→97.9	61.5	38.5	93.4→93.8	75.0	93.8	99.3→ 100	100
stage 3	89.5→96.2	100	100	99.6→ 100	100	75.0	99.3→ 100	84.6
	Total horizon: 6,500 h→6,294 h			Total horizon: 6,500 h→6,492 h			Total horizon: 6,500 h→6,467 h	

Problem size: 1,824 var.(744 bin.var.); 3,985 const., solved in 764.5 s

5. Conclusion

In this paper, the design of a chemical batch plant equipped with parallel production lines is studied. We have introduced parallel lines as a strategic design option into existing multiproduct sequential design models and formulated a mathematical model so as to minimise costs. These parallel lines are specific lines over which total production will be divided and that may be dedicated to particular products or product families. Concerning the objective function, we introduced, besides capital costs, also startup, contamination and operating costs. We illustrated our model with an example, where not only the number and size of the equipment, but also the number of parallel lines and the assignment of products to the installed lines had to be determined. The results indicate that the presence of parallel lines allows for a reduction in total costs

as not all products have to share all equipment any more, leading to smaller (bottleneck) equipment and lower startup costs. Also, the dedication of these lines to product families lowers total setup costs by avoiding high contamination costs. Furthermore, while minimising operating costs, volume-wise asset utilisation is optimised within the bounds of the optimal equipment sizes. This generates spare time, which can be used as a small time buffer improving reliability. In future research, we will investigate other modes of operation, as opposed to single product campaigns, in order to reflect a more realistic operational use. Furthermore, we will look into other business objectives besides cost effectiveness.

Appendices

Appendix A. Nomenclature

Table A.1: Nomenclature.

Indices	
i	products (P)
j	stages (J)
l	lines (L)
s	discrete sizes (S)
n	number of equipment in parallel (N)
Parameters	
S_{ij}	size factor of product i in stage j
τ_{ij}	processing time of product i in stage j
Q_i	total amount to produce of product i
H	horizon, total available production time
v_s	tank size s
M_i	upper bound on number of batches of product i
α_j, β_j	cost coefficients of stage j
d_{if}	boolean matrix indicating if product i belongs to family f
c_{js}	capital costs of stage j with size s ($\alpha_j v_s^{\beta_j}$)
$Cstart_i$	startup costs of product i

C_{cont}	fixed contamination cost between product families
C_{operat_i}	operating cost of product i

Variables

Continuous:

q_{li}	amount produced of product i on line l
n_{li}	number of batches of product i on line l
T_{lji}	total time spent on product i on stage j of line l
θ_{li}	total time spent on product i on line l
Z_{ljis}	product of q_{li} and u_{ljs} (linearisation)
X_{ljin}	product of T_{lji} and z_{ljn} (linearisation)

Binary:

z_{ljn}	if unit n of stage j of line l exists
t_{li}	if product i is produced on line l
u_{ljs}	if stage j of line l has units of size s
b_{fl}	if product family f is produced on line l
g_l	if there are more than 1 product families on line l (correction term)
Y_{ljsn}	product of u_{ljs} and z_{ljn} (linearisation)
V_{ljin}	product of t_{li} and z_{ljn} (linearisation)
U_{ljfn}	product of b_{fl} and z_{ljn} (linearisation)
H_{ljfn}	product of U_{ljfn} and g_l (linearisation)

400 Appendix B. Visual overview of the example

Figure B.1: Overview design decisions for a single line with (possible) parallel equipment per stage, including different cost components

Figure B.2: Overview design decisions for parallel lines as a decision variable, with (possible) parallel equipment per stage, including different cost components

Acknowledgements

This work was supported by the Research Foundation - Flanders (FWO).

References

- Applequist G, Samikoglu O, Pekny J, Reklaitis G. Issues in the use, design and evolution of process scheduling and planning systems. *ISA Trans* 1997;36(2):81 – 121.
- Barbosa-Póvoa AP. A critical review on the design and retrofit of batch plants. *Comp Chem Eng* 2007;31(7):833 –55.
- Barbosa-Póvoa AP, Macchietto S. European symposium on computer aided process engineering- detailed design of multipurpose batch plants. *Comp Chem Eng* 1994;18(11):1013 –42.
- Barbosa-Póvoa AP, Pantelides CC. Design of multipurpose plants using the resource-task network unified framework. *Comp Chem Eng* 1997;21, Supplement:S703 –8.
- Biegler LT, Westerberg AW, Grossmann IE. Systematic methods of chemical process design. Upper Sadle River, N.J., Pearson, 1997.

- Birewar DB, Grossmann IE. Incorporating scheduling in the optimal design of multiproduct batch plants. *Comp Chem Eng* 1989;13(1–2):141–61. *Computer Applications to Batch Chemical Processing*.
- 420 Birewar DB, Grossmann IE. Simultaneous synthesis, sizing, and scheduling of multiproduct batch plants. *Ind Eng Chem Res* 1990;29(11):2242–51.
- Castro PM, Barbosa-Póvoa AP, Novais AQ. Simultaneous design and scheduling of multipurpose plants using resource task network based continuous-time formulations. *Ind Eng Chem Res* 2005;44(2):343–57.
- 425 Cerdá J, Henning GP, Grossmann IE. A mixed-integer linear programming model for short-term scheduling of single-stage multiproduct batch plants with parallel lines. *Ind Eng Chem Res* 1997;36(5):1695–707.
- Chen CL, Liu CL, Feng XD, Shao HH. Optimal short-term scheduling of multiproduct single-stage batch plants with parallel lines. *Ind Eng Chem Res* 430 2002;41(5):1249–60.
- Corsano G, Montagna JM, Iribarren OA, Aguirre PA. Heuristic method for the optimal synthesis and design of batch plants considering mixed product campaigns. *Ind Eng Chem Res* 2007;46(9):2769–80.
- Dietz A, Azzaro-Pantel C, Pibouleau L, Domenech S. Multiobjective optimization for multiproduct batch plant design under economic and environmental 435 considerations. *Comp Chem Eng* 2006;30(4):599–613.
- Floudas CA, Lin X. Continuous-time versus discrete-time approaches for scheduling of chemical processes: a review. *Comp Chem Eng* 2004;28(11):2109–29.
- 440 Fumero Y, Corsano G, Montagna JM. A mixed integer linear programming model for simultaneous design and scheduling of flowshop plants. *Appl Math Model* 2013;37(4):1652–64.

- Goel HD, Grievink J, Weijnen MPC. Integrated optimal reliable design, production, and maintenance planning for multipurpose process plants. *Comp Chem Eng* 2003;27(11):1543–55.
- Gooding WB, Pekny JF, McCroskey PS. Enumerative approaches to parallel flowshop scheduling via problem transformation. *Comp Chem Eng* 1994;18(10):909–27.
- Grossmann IE, Sargent RWH. Optimum design of multipurpose chemical plants. *Ind Eng Chem Proc Des Dev* 1979;18(2):343–8.
- Gurobi . Gurobi optimizer reference manual. Gurobi Optimization Inc.; 6th ed.; 2016. .
- Harjunkski I, Maravelias CT, Bongers P, Castro PM, Engell S, Grossmann IE, Hooker J, Méndez C, Sand G, Wassick J. Scope for industrial applications of production scheduling models and solution methods. *Comp Chem Eng* 2014;62:161–93.
- Hill A, Cornelissens T, Sørensen K. Efficient multi-product multi-bom batch scheduling for a petrochemical blending plant with a shared pipeline network. *Comp Chem Eng* 2016;84:493–506.
- Jelen FC, Black JH, of Cost Engineers AA. Cost and optimization engineering. McGraw-Hill, 1983.
- Knopf FC, Okos MR, Reklaitis GV. Optimal design of batch/semicontinuous processes. *Ind Eng Chem Proc Des Dev* 1982;21(1):79–86.
- Kondili E, Pantelides CC, Sargent RWH. A general algorithm for short-term scheduling of batch operationsi. milp formulation. *Comp Chem Eng* 1993;17(2):211–27.
- Lamba N, Karimi IA. Scheduling parallel production lines with resource constraints. 1. model formulation. *Ind Eng Chem Res* 2002;41(4):779–89.

- Lin X, Floudas CA. Design, synthesis and scheduling of multipurpose batch
470 plants via an effective continuous-time formulation. *Comp Chem Eng*
2001;25(46):665–74.
- Loonkar YR, Robinson JD. Minimization of capital investment for batch pro-
cesses. calculation of optimum equipment sizes. *Ind Eng Chem Proc Des Dev*
1970;9(4):625–9.
- 475 Méndez CA, Cerdá J, Grossmann IE, Harjunkski I, Fahl M. State-of-the-art
review of optimization methods for short-term scheduling of batch processes.
Comp Chem Eng 2006;30(6–7):913–46.
- Méndez CA, Henning GP, Cerdá J. An milp continuous-time approach to short-
term scheduling of resource-constrained multistage flowshop batch facilities.
480 *Comp Chem Eng* 2001;25(4–6):701–11.
- Modi AK, Karimi IA. Design of multiproduct batch processes with finite inter-
mediate storage. *Comp Chem Eng* 1989;13(1–2):127–39.
- Moreno MS, Montagna JM. New alternatives in the design and planning of
multiproduct batch plants in a multiperiod scenario. *Ind Eng Chem Res*
485 2007;46(17):5645–58.
- Pinto JM, Grossmann IE. A continuous time mixed integer linear programming
model for short term scheduling of multistage batch plants. *Ind Eng Chem*
Res 1995;34(9):3037–51.
- Pinto T, Barbosa-Póvoa AP, Novais AQ. Optimal design and retrofit of batch
490 plants with a periodic mode of operation. *Comp Chem Eng* 2005;29(6):1293
–303.
- Pistikopoulos EN, Thomaidis TV, Melin A, Ierapetritou MG. Flexibility, relia-
bility and maintenance considerations in batch plant design under uncertainty.
Comp Chem Eng 1996;20, Supplement 2:S1209–14. European Symposium
495 on Computer Aided Process Engineering.

- Rippin DWT. Design and operation of multiproduct and multipurpose batch chemical plants. an analysis of problem structure. *Comp Chem Eng* 1983;7(4):463–81.
- Seid ER, Majozi T. Design and synthesis of multipurpose batch plants using a robust scheduling platform. *Ind Eng Chem Res* 2013;52(46):16301–13.
- Sparrow RE, Forder GJ, David WT. The choice of equipment sizes for multiproduct batch plants. heuristics vs. branch and bound. *Ind Eng Chem Proc Des Dev* 1975;14(3):197–203.
- Takamatsu T, Hashimoto I, Hasebe S. Optimal design and operation of a batch process with intermediate storage tanks. *Ind Eng Chem Proc Des Dev* 1982;21(3):431–40.
- Voudouris VT, Grossmann IE. Mixed-integer linear programming reformulations for batch process design with discrete equipment sizes. *Ind Eng Chem Res* 1992;31(5):1315–25.
- Xia Q, Macchietto S. Supplement to computers and chemical engineering design and synthesis of batch plants minlp solution based on a stochastic method. *Comp Chem Eng* 1997;21:S697–702.