Computers and Chemical Engineering 177 (2023) 108341

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/cace

A time-bucket MILP formulation for optimal lot-sizing and scheduling of real-world chemical batch plants

R. Wallrath [a,c,*], F. Seeanner [b], M. Lampe [a], M.B. Franke [c]

[a] Bayer AG, Kaiser-Wilhelm Allee 1, 51368 Leverkusen, Germany
[b] SimPlan Systems GmbH, Sophie-Scholl-Platz 6, 63452 Hanau, Germany
[c] University of Twente, Faculty of Science and Technology, Sustainable Process Technology, Process Design and Optimization, Drienerlolaan 5, 7522 NB Enschede, The Netherlands

ARTICLE INFO

Keywords:
Mixed-integer linear programming
Time-bucket formulation
Lot-sizing and scheduling
Chemical batch plants
Flow shop optimization
Multi-stage manufacturing process

ABSTRACT

We propose a new time-bucket MILP model for lot-sizing and scheduling problems arising in chemical batch plants. The main idea behind time-bucket models is to partition time into fixed-length macroperiods and flexible length microperiods, that lie within the macroperiods. We show that the time-bucket model benefits from advantages of both continuous and discrete time representations. It allows to include important real-world constraints, can be solved with moderate computational effort, and thus promotes MILP for large-scale, industrial problems. We investigate the scalability of the model and apply it to a formulation and filling process from an industrial agrochemical production with 7 formulation lines, intermediate buffer tanks, and 7 filling lines. We optimize a one month period with 50 intermediates, and 83 finished products. A comparison of the MILP solution to a discrete event simulation solution shows that 17% of production capacity can be freed up and significant improvement in on-time delivery.

1. Introduction

Production scheduling of large-scale, industrial processes is widely recognized as a challenging optimization task both by academic and industrial researchers. With an increasing availability of real-time process data, ever-growing computational capabilities, and the advance of digital twins, optimal production scheduling has gained new relevance. However, there is still a large gap between industrial reality and academic research. As pointed out in Harjunkoski (2016), practitioners are confronted with many different challenges, when building their solutions in an industrial environment. While mixed-integer programming (MIP) is a well established optimization technique in asset-heavy industries such as petrochemicals (Castro et al., 2018) and discrete manufacturing industries such as semiconductors (Qin et al., 2019) and automotive (Gnoni et al., 2003), it is relatively new to industries such as specialty chemicals (Borisovsky et al., 2019), pharma (Sarin et al., 2014; Costa, 2015), and consumer goods (Sel et al., 2015; Clark et al., 2011). New, industry-specific requirements for scheduling solutions arise, which have to be harmonized with the natural drawbacks of MIP: Since MIP models suffer from the curse of dimensionality, they are limited in modeling depth and quickly grow to intractable size. However, optimal decisions in real-world production environments require sufficiently detailed models. In addition, setting up and maintaining MIP models is a difficult task as model formulations often are abstract and hard to understand intuitively. Alternatives such as discrete event simulation (DES) allow high-fidelity modeling and fast solution times, but do not provide bounds on the solutions. Therefore the quality of simulation results can only be assessed by applying exhaustive search strategies, for instance by exploring sets of dispatching rules. Optimality criteria to terminate the solution process prematurely cannot be used with DES. Despite extensive research efforts with MIP and DES (Castro et al., 2011; Frazzon et al., 2016; Nikolopoulou and Ierapetritou, 2012), real-world scheduling problems with dozens of products and machines, secondary resources, changeover costs, and lot-sizing still can only be solved sub-optimally or require massive computational resources.

Herein we propose a new time-bucket mixed-integer linear programming (MILP) model for lot-sizing and scheduling problems arising in multistage production processes. The main idea behind time-bucket models is to partition time into fixed-length macroperiods and flexible length microperiods, that lie within the macroperiods. This model formulation allows to include important real-world constraints and can be solved with moderate computational resources.

To investigate the properties of the proposed time-bucket formulation we run 50 random instances for different model configurations,

* Corresponding author at: University of Twente, Faculty of Science and Technology, Sustainable Process Technology, Process Design and Optimization, Drienerlolaan 5, 7522 NB Enschede, The Netherlands.
E-mail address: r.wallrath@utwente.nl (R. Wallrath).

https://doi.org/10.1016/j.compchemeng.2023.108341
Received 26 March 2023; Received in revised form 4 June 2023; Accepted 25 June 2023
Available online 1 July 2023

and discuss solution time as well as convergence of the bounds. Subsequently, we apply our approach to a real-world case study of a large-scale industrial make-and-fill process of an agrochemical production plant. We show that our modeling approach is able to capture the different characteristics of the problem efficiently and provides near-optimal schedules of a 1-month production data set with moderate computational effort. To validate the MILP results, we reconcile them with a validated DES model of the process. We then compare the resulting schedule to the real production schedule, which was developed by production experts using the DES model only.

The rest of the article is structured as follows: In Section 2 we provide a problem classification, and an overview of the recent literature. In Section 3 we describe the generic flow shop MILP model, the two-step solution procedure, and introduce the terminology. In Section 4 we discuss the scalability of the model. We analyze solution times and the convergence of upper and lower bound for different model configurations. In Section 5 we discuss a real-world case study. We introduce the make-and-fill process of an agrochemical production plant and apply our modeling approach to a one-month production period. Thereafter, we reconcile the MILP results with a validated DES model of the process and compare the reconciled result to a real-word production plan. In Section 6 we give a conclusion and an outlook for future work.

2. Literature

2.1. General classification

Scheduling problems are traditionally classified by the triplet α / β / γ, where α stands for the machine environment, β for the processing characteristics and constraints and γ for the choice of the objective function (Pinedo, 2008). Accordingly, we introduce our scheduling problem as (α) a flexible flow shop with (β) sequence-dependent setup times, machine availability and eligibility constraints given the objectives (γ) of total weighted tardiness minimization and changeover cost minimization.

The authors of Méndez et al. (2006) suggest a detailed classification of batch scheduling problems with respect to the (1) process topology, (2) equipment assignment, (3) equipment connectivity, (4) inventory storage policies, (5) material transfer, (6) batch size, (7) batch processing time, (8) demand patterns, (9) changeovers, (10) resource constraints, (11) time constraints, (12) cost, and (13) degree of certainty. In this framework our problem classifies as a (1) multistage flowshop with (2) variable equipment assignment, (3) restricted equipment connectivity, (4) finite, shared intermediate storage, (5) instantaneous material transfer, (6) variable batch size, (7) product-, equipment-, and batchsize dependent processing time, (8) multiproduct demand with multiple due dates, (9) sequence- and equipment-dependent changeover times, (10) discrete equipment and personnel resource constraints, (11) individual shift schedules per stage, (12) backlog and changeover costs, that is (13) deterministic.

In addition to these two classifications, the authors of Georgiadis et al. (2019) highlight the importance of (1) the optimization decisions, and (2) time representation, which we will review in the following sections.

2.2. Optimization decisions: Simultaneous lot-sizing and scheduling

Optimization decisions refer to the decision variables of a model and are directly related to model depth and solution effort. While scheduling is the task of selecting a product, a processing resource and the timing of production, lot-sizing is the task of defining the batch size or the quantity of a production campaign. This additional degree of freedom adds significant complexity to conventional scheduling problems because continuous variables are introduced, that must be taken into account by the time representation. Simultaneous lot-sizing and scheduling is an active research area in the operations research and process system engineering community. We review the state-of-the art of problem formulations and solution approaches as well as use cases in the following.

In operations research, especially in supply chain management and logistics, simultaneous lot-sizing and scheduling have been studied over a long time. The multi-level capacitated lot-sizing problem (MLCLSP) (Tempelmeier and Helber, 1994) describes interactions of lot-sizing decisions across multiple, capacity-constrained production stages. The authors of Meyr (2004) define the generalized lot-sizing and scheduling problem for multiple production stages (GLSPMS). The authors of Seeanner and Meyr (2013) suggest several enhancements to this framework to make it more flexible for different problem settings of the consumer packaged goods industry. A recent overview of lot-sizing and scheduling with resource constraints can be found in Wörbelauer et al. (2019).

Due to the model complexity, the application of deterministic mathematical optimization algorithms lead to prohibitive solutions times. Instead, heuristic or meta-heuristic solution approaches are being used frequently. In Berretta et al. (2005) a multilevel lot-sizing problem with general product structures, setup times, and lead times is solved using heuristics to find good solutions efficiently. Tabu search with simulated annealing components are adopted to refine the solutions. In Toledo et al. (2013) a hybrid multi-population genetic algorithm applied to solve the multi-level capacitated lot-sizing problem with backlogging. In Wu et al. (2013), a MIP formulation for an instance of the same problem as in Toledo et al. (2013) is adopted and a solution algorithm based on temporal decomposition is suggested. The authors of Qin et al. (2019) use ant-colony optimization in a two-state solution procedure to address a flow-shop scheduling problem with lot-sizing and calendar constraints in printed circuit board assembly. The authors of Clark et al. (2011) consider a lot-sizing and scheduling problem with sequence-dependent changeover times of an animal nutrition plant as an asymmetric traveling salesman problem and propose an iterative solution approach based on subtour elimination and patching steps.

In the process system engineering community, different real-world case studies have recently been solved.

In Elzakker et al. (2012), a short-term scheduling problem arising from a multiproduct, mix-and-pack process in the fast-moving consumer goods industry is solved. The authors adopt a unit-specific continuous time representation and additionally define dedicated time intervals, which only allow specific groups of products to be produced. Furthermore, the time intervals of the mixing and packing stage are coupled to model the intermediate buffers efficiently. However, with 8 products and only one mixing and two packaging lines the problem size is limited.

In Georgiadis et al. (2020), a multistage real-life food processing plant with 35 products and sequence-dependent changeover times is considered. The authors reduce model complexity by reformulating a production stage, that consists of batch processing units and cannot become the bottleneck, as a simpler resource constraint. The problem is solved by a decomposition approach in which the products to be scheduled are optimized iteratively, which has the disadvantage that the order between already scheduled products is fixed and may lead to suboptimal solutions. In Basán et al. (2019), an efficient MILP-based decomposition strategy is introduced to solve a flexible flow shop problem arising from the two-stage discrete manufacturing process of vessels for the offshore oil and gas industry. Instead of tackling the full problem size at once, first, in a solution construction phase, all jobs are successively inserted into a schedule that is then re-optimized every time. Secondly, in a solution improvement phase, all jobs are successively rescheduled until no improvement is achieved.

In Elekidis and Georgiadis (2021), a make-and-pack process with intermediate buffer from the consumer goods industry is formulated as a continuous-time, precedence-based MILP. The authors present a high granular process model featuring explicit mass balances of the intermediate storage vessels and byproduct capacity constraints. They propose an order-based decomposition method, in which subsets of orders are successively inserted in a constructive solution step, and then re-inserted into the schedule in an improvement step.

Although different real-world problems have been solved recently, the contributions also show that great improvement potential in terms of efficient model formulations and solution procedures exist. Most of the contributions decompose the original problem to obtain a tractable problem size. However, we aim to schedule all products (orders) at once, that means, monolithically, without any order-based decomposition or similar heuristics.

2.3. Time representation

The aspect of time representation is of fundamental importance for an efficient model formulation. The concepts of discrete versus continuous time representation (Floudas and Lin, 2004) are well established and have been developed further in numerous examples (Klanke et al., 2021; Lee and Maravelias, 2018). While a discrete time representation requires a large number of variables to define fixed, equal-length time intervals, a continuous time representation usually requires less variables to define flexible, variable-length time intervals. On the other hand, the continuous time approach usually comes with precedence variables, global or unit-specific event points and constraints to enforce the chronology of time intervals. Although time representation has been extensively studied in the context of process representation concepts such as the state-task network (STN) (Kondili et al., 1993; Maravelias and Grossmann, 2003) and resource-task network (RTN) (Pantelides, 1994; Schilling and Pantelides, 1996) it remains an active topic of research. For instance, in Castro (2022), the challenging scheduling problem of a multiproduct batch chemical plant featuring sequence-dependent changeovers and their possibility to be interrupted, alternative recipes, and unstable intermediates is solved to optimality using a discrete-time RTN formulation.

Continuous-discrete time representations benefit from the advantages of both continuous and discrete time formulations while overcoming their shortcomings. To this end, authors suggest to embed a discrete time grid into a continuous time frame, or vice versa.

The authors of Georgiadis et al. (2020) model the main production decisions in a continuous timeframe and map the resulting allocation of resources onto a discrete time grid. An order-decomposition approach is used to solve the MILP model. In Kopanos et al. (2011), a similar multistage diary production process is modeled using a discrete-continuous time representation. The discrete time grid consists of 1-production-day intervals, on which mass balances are enforced. Within each interval operations are scheduled in continuous time. There are 23 product families considered and the model is solved in a monolithical fashion. The production of each product family must be finished at the end of the day and is not allowed to reach over to the next production day. In Seeanner and Meyr (2013), a micro-macro-period time structure is proposed for the multi-stage lotsizing and scheduling problem. The structure is based on variable-length small time buckets in which different operations take place, and fixed-length big-time buckets which enforce material balance equations and resource constraints. The model allows operations to be split across consecutive big-time buckets to obtain a tighter problem formulation. The authors suggest different solution methods such as relax-and-fix and heuristic approaches. In Lee and Maravelias (2018), a sequential discrete-continuous time representation is proposed. First, a discrete time model is solved to obtain an approximate solution quickly. The solution is mapped onto a continuous time model, which is then solved again. The authors study literature scheduling problems and solve both the discrete and continuous time model monolithically.

In this paper, we follow the time bucket approach from Seeanner and Meyr (2013) and embed continuous time intervals (microperiods) into a discrete time grid (macroperiods). We extend the approach of Seeanner and Meyr (2013) by adding real-world constraints like personnel and shift constraints as well as batch size and shelf life constraints which are required for chemical batch process scheduling. Together with the developed monolithic 2-step solution approach, we show that we obtain feasible, near-optimal solutions in reasonable solutions times.

3. Problem statement

3.1. Illustrative example

We illustrate the task of simultaneous lot-sizing and scheduling using a 2-stage chemical process. The lot-sizing task is to define optimal lot sizes, that is, the lengths of uninterrupted production campaigns of specific products. At the same time the scheduling task is to find the optimal timing for these lots given changeover costs, due dates and other constraints. Simultaneous lot-sizing and scheduling for multistage processes with multiple processing resources per stage and intermediate storage is particularly complex. Lot sizes and schedules in each stage must be synchronized by mass balances, while lots may be split up when transferring from one stage to the next. Operator resources may limit the number of processing resources that are available simultaneously. Product and resource specific production rates as well as sequence-dependent changeover times exist. In hybrid environments, one intermediate product can be converted into different finished products. Therefore production decision must be made taking into account the due dates.

An example of a 2-stage process is shown in Fig. 2. For simplicity, we assume 1 line per stage and 1 buffer unit exist. In stage 1 two different bulk products A, and B are produced each of which yields two different finished products A1, A2, B1, and B2 in stage 2. Sequence-dependent changeover times in stage 1 from product i to product j are assumed. Furthermore, we assume a demand of 2 finished products associated with due date 1 and 3 finished products associated with due date 2. The task of lot-sizing and scheduling is to define lots for stage 1 and 2 and to schedule them in such a way that backlog is avoided. We use the term backlog to refer to produced quantities that violate due dates. In addition, we define the minimization of changeover times as objective function. In the illustrative example, we assume that the changeover times cause stage 1 to be the bottleneck. In the proposed schedule to avoid backlog by due date 1, product A must be produced before product B in stage 1. This however causes long changeover times when switching back to product A. Therefore, large lot sizes of bulk product A, which can be stored in the buffer unit for later release into stage 2, are preferable. Since the buffer unit is limited in capacity additional bulk product A has to be produced to satisfy the demand of finished products A1 and A2 associated with due date 2.

The example shows that lot-sizing and scheduling for multi-stage systems is a difficult task with many sources of complexity, which consequently must be included in optimization models. Since time representation is the cornerstone for precise and efficient model formulations, we introduce the time-bucket model in the following.

3.2. Time formulation

In the time-bucket model, we combine the advantages of a flexible and a fixed time grid to efficiently model challenging constraints. While mass balances, resource allocations, shift schedules, and due dates are modeled in the fixed time grid, production quantities and changeover times are modeled in the flexible time grid. The fixed time grid consists of marcoperiods, while the flexible time grid consists of microperiods. Macroperiods are fixed time intervals with uniform length, that are defined globally. As shown in Fig. 1, there is the same fixed number of microperiods $s \in S_t$ in each macroperiod $t \in T$. The number of microperiods can be adjusted to achieve the desired modeling depth. Microperiods are flexible time intervals with variable length, that are

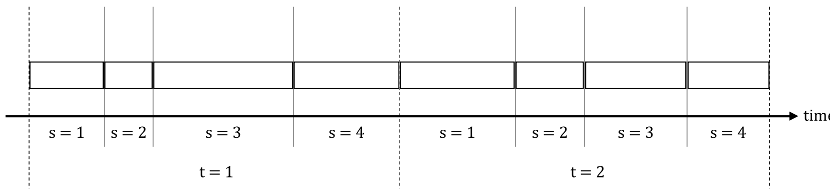


Fig. 1. Time representation example of 2 macroperiods each featuring 4 microperiods.

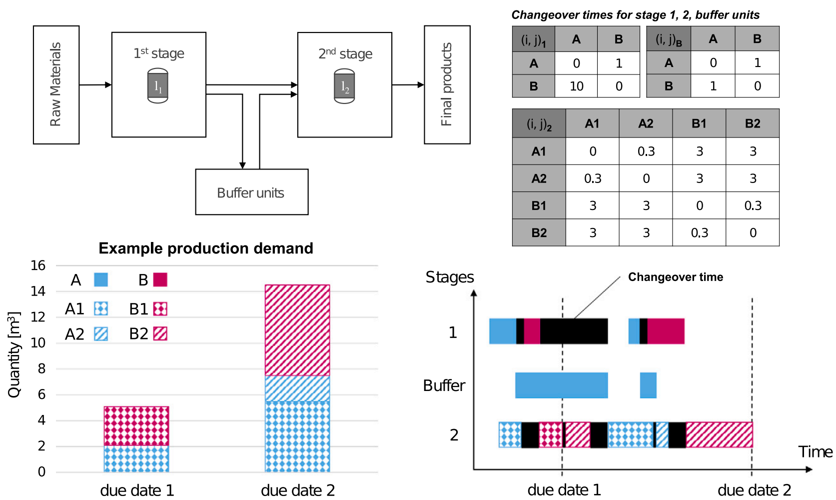
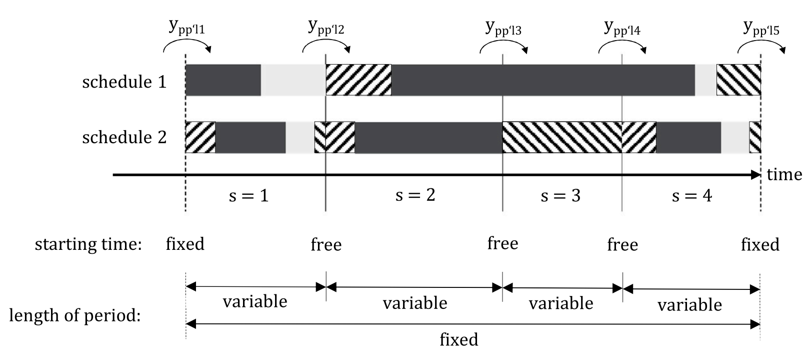


Fig. 2. Simultaneous lotsizing and scheduling for a 2-stage example process with intermediate buffer.

(a) Microperiods consist of setup start, production, idle and setup end phase.



(b) 2 possible schedules on a resource l in 1 macroperiod with 4 microperiods s.

Fig. 3. Micro- and macroperiods provide a flexible time structure to model different production modes.

defined per processing resource. Since microperiods have a variable length, one microperiod can cover a full macroperiod, which implies that the other microperiods in this macroperiod have lengths of 0. Binary changeover variables $y_{pp'ls}$ indicate changeovers from product p to p' on processing resource l in microperiod s. Each microperiod consists of a fixed sequence of 4 phases, *set-up start*, *production*, *idle*, and *set-up end* as shown in Fig. 3(a).

The variable lengths of the phases are determined by the product and quantity in the microperiod. The length of phase *production* is determined by the lot size and the lengths of phases *set-up start* and *set-up end* are determined by the changeover time. Phase *idle* provides an optional idle interval. We consider the example of a processing resource l in a macroperiod with 4 microperiods as shown in Fig. 3(b). In $schedule1$ two production phases take place. In this case, p is equal to p' for both $y_{pp'l3}$, and $y_{pp'l4}$. The same time structure also allows to model 3 production phases as shown in $schedule2$. The changeover times must be taken into account using the *setup start* and *setup end* phases. In this case, the changeover from product p in microperiod $s = 2$ to product p' in microperiod $s = 4$ requires a changeover time that covers microperiod $s = 3$ fully. Generally, this time formulation allows,

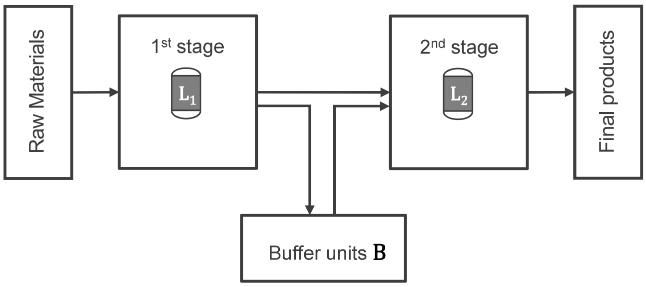


Fig. 4. 2-stage flow shop process with parallel processing resources per stage L_i and intermediate buffer units B.

that the *production* phase can cover full microperiods if no changeover time is required. Similarly, long changeover times and idle times can be modeled. Since the microperiods are defined per processing resource l and have variable lengths, the time bucket approach provides a highly flexible time representation to our model.

3.3. General plant setup

We consider the lot-sizing and scheduling problem arising from a multistage, flexible flow shop environment with product sequence and processing resource dependent changeover times, finite intermediate storage and personnel constraints given the objective to minimize the total changeover time and backlog quantities. As shown in Fig. 4, raw materials are processed in 2 process stages, each consisting of L_i processing resources. The materials can optionally be stored B buffer units between the process stages. Each processing resource can be seized by one product at a time and sequence- as well as resource-dependent changeover times are assumed. In addition, there are minimum batch sizes for the first stage resources, which are product- and resource-specific. The demand is defined with respect to the final products. We consider different shift schedules for the process stages. The shift schedules determine the maximum number of lines that can be in the production or set-up phase at the same time due to the availability of operators. Lastly, we generally assume that transfer times of quantities from one stage to another are negligible compared to processing and changeover times.

3.4. Problem formulation

We specify the sets, variables and parameters of our model in Table 1. The variables reflect key decision aspects of (1) product, and resource selection as well as lot-sizing, (2) product sequencing, (3) product conversion from intermediates to finished products, and (4) personnel allocation. In addition, we define input parameters such as product demands with due dates, sequence dependent changeover times, product and resource specific run rates, bill of material coefficients, minimum lot sizes, limits of operating capacity per stage, limited inventory and backlog capacities, and others.

Objective function and solution procedure. We chose the minimization of backlog and changeover times as the objective. A traditional 1-step, monolithic solution approach that solves the full model for the final objective at once can lead to long computing times. We suggest a 2-step, monolithical solution approach with warm start to optimize backlog and changeover times sequentially. In the first optimization step, we define the minimization of all backlog quantities $B_{\hat{p}t}$ as the objective as shown in Eq. (1). In contrast, a multi-step, polylithical approach solves parts of the model sequentially, which is faster but can be difficult to set up and influence solution quality, as discussed in Section 2.2.

$$\min \sum_{\hat{p} \in \mathbb{FP}} \sum_{t \in T} B_{\hat{p}t} \tag{1}$$

Table 1
Description of sets, variables and parameters used in the model.

Set	Description
T	Set of macroperiods, indexed $t \in T$
S_t	Set of microperiods in macroperiod t, indexed $s \in S$
$\mathbb{IP}$	Set of intermediate products, indexed $p \in \mathbb{IP}$
$\mathbb{FP}$	Set of finished products, indexed $\hat{p} \in \mathbb{FP}$
$\mathbb{P}$	Union of $\mathbb{IP}$ and $\mathbb{FP}$, indexed $p \in \mathbb{P}$
$\mathbb{L}_i$	Set of all processing resources in stage i indexed $l \in \mathbb{L}_i$
$\mathbb{L}$	Union of all $\mathbb{L}_i$ across stages, indexed $l \in \mathbb{L}$
Variable	**Description**
Continuous	
q_{pls}	Quantity of a production order of product p on resource l in microperiod s
I_{pt}	Inventory of a product p at the end of macroperiod t
$B_{\hat{p}t}$	Backlog quantity of product p at the end of macroperiod t
$h_{start,ls}$	Duration of *setup start* phase on resource l in microperiod s
$h_{end,ls}$	Duration of *setup end* phase on resource l in microperiod s
$h_{idle,ls}$	Duration of *idle* phase on resource l in microperiod s
k_{ls}	Start time of microperiod s on resource l
Discrete	
$y_{pp\prime ls}$	Binary changeover variable indicating a product switch from product p in microperiod $s-1$ to product p' in microperiod s on resource l
o_{lt}	Binary variable indicating whether there is no sufficient personnel in macroperiod t to operate resource l
Parameter	**Description**
$D_{\hat{p}t}$	Quantity of finished product $\hat{p}$ that is demanded at the end of macroperiod t
$ct_{pp\prime l}$	Changeover time between product p and p' on processing resource l. Changeover time for $p = p'$ is 0.
a_{pl}	Production coefficients expressing the processing time for 1 volumetric unit of product p on resource l. The coefficients depend on the product viscosity and the milling efficiency of the processing resource.
$b_{p\hat{p}}$	Bill of material coefficients that describe the conversion options of intermediate product p into finished product $\hat{p}$
C_{max}	Fixed length of one macroperiod
$F^i_{max,t}$	Staffing level in stage i during macroperiod t determining the maximum number of processing resources that can be operated simultaneously
I^{max}	Maximum total quantity of all intermediate products that can be stored as inventory between process stages
$q_{min,l}$	Minimum lotsize on processing resource l
γ	Maximum number of microperiods in which quantities must be unloaded from inventory
$B_{\hat{p},max}$	Maximum backlog quantity of finished product $\hat{p}$
λ	Fixed number of microperiods in which the minimum lot size must be realized.

The second optimization step is initialized with the results of the first step. In particular, the binary changeover variables $y_{pp\prime ls}$, which denote the product-resource allocations, are initialized with the result of the first step. In addition, an upper bound constraint for the total backlog is added. The maximum allowed total backlog is enforced to be less or equal than the objective value found in the first step, as shown in Eq. (17). The objective of the second step is the minimization of the total changeover time $y_{pp\prime ls} ct_{pp\prime l}$ as shown in Eq. (2).

$$\min \sum_{t \in T} \sum_{s \in S_t} \sum_{l \in \mathbb{L}} \sum_{p,p\prime \in \mathbb{P}} y_{pp\prime ls} ct_{pp\prime l} \tag{2}$$

Inventory balance for intermediate products. As shown in Eq. (3) the inventory I_{pt} of an intermediate product $p \in \mathbb{IP}$ in macroperiod $t \in T$ is calculated from the inventory in the previous macroperiod I_{pt-1}, all produced quantities q_{pls} of intermediate p on resources $l \in L_1$ during the microperiods $s \in S_t$ and all consumed quantities $b_{p\hat{p}} q_{\hat{p}ls}$ of intermediate p on resource $l \in L_2$ during microperiods $s \in S_t$. The inventory balance for intermediate products is enforced for all macroperiods.

$$I_{pt} = I_{pt-1} + \sum_{l \in L_1} \sum_{s \in S_t} q_{pls} - \sum_{\hat{p} \in \mathbb{FP}} \sum_{l \in L_2} \sum_{s \in S_t} b_{p\hat{p}} q_{\hat{p}ls} \qquad \forall p \in \mathbb{IP}, t \in T \quad (3)$$

Inventory balance for finished products. As shown in Eq. (4) the inventory $I_{\hat{p}t}$ of a finished product $\hat{p} \in \mathbb{FP}$ in macroperiod $t \in T$ is calculated from the inventory in the previous macroperiod $I_{\hat{p}t-1}$, all produced quantities $q_{\hat{p}ls}$ for product $\hat{p}$ on resources $l \in L_2$ during microperiods $s \in S_t$, the demand quantities $D_{\hat{p}t}$, and the backlog quantities $B_{\hat{p}t}$, and $B_{\hat{p}t-1}$ in the current and previous macroperiod. Since inventory levels cannot be negative, $D_{\hat{p}t}$ ensures the minimum demand quantity is kept in stock at the demand date. This demand satisfaction is relaxed by backlog variables $B_{\hat{p}t}$, and $B_{\hat{p}t-1}$. If positive, the backlog $B_{\hat{p}t}$ represents delayed quantity of product $\hat{p}$ in macroperiod t. $B_{\hat{p}t}$ is added to the right-hand side of Eq. (4) to compensate the deficit of the demand $D_{\hat{p}t}$, inventory $I_{\hat{p}t-1}$, and the produced quantities $q_{\hat{p}ls}$. At the same time, the backlog $B_{\hat{p}t-1}$ from the previous macroperiod must be substracted on the right-hand side of Eq. (4). If positive, $B_{\hat{p}t-1}$ represents the deficit that is carried over from the previous macroperiod. The inventory balance for finished products is enforced for all macroperiods.

$$I_{\hat{p}t} = I_{\hat{p}t-1} + \sum_{s \in S_t} \sum_{l \in L_2} q_{\hat{p}ls} - D_{\hat{p}t} + B_{\hat{p}t} - B_{\hat{p}t-1} \qquad \forall \hat{p} \in \mathbb{FP}, t \in T \qquad (4)$$

Changeover constraint. We assume an unique setup state of a resource in a microperiod, that is determined by the running product. Consequently, a changeover between two setup states takes place when switching products in subsequent microperiods. The binary changeover variable $y_{pp\prime ls}$ is an indicator of a transition between setup states of products p and $p\prime$ on line l in microperiod s. The corresponding changeover time will be imposed based on $y_{pp\prime ls}$. As shown in Eq. (5), the changeover variable must be equal to 1 for a specific product pairs $pp\prime$, which means that a unique setup state must exist in each microperiod and on each resource. The constraint is imposed on all microperiods S_t of all macroperiods $t \in T$.

$$\sum_{p \in \mathbb{P}} \sum_{p\prime \in \mathbb{P}} y_{pp\prime ls} = 1 \qquad \forall l \in \mathbb{L}, s \in S_t, t \in T \qquad (5)$$

Enforce setup constraint. Production of $p \in \mathbb{P}$ can only take place on a processing resource $l \in \mathbb{L}$ if the resource is set up for this product in microperiod s. As shown in Eq. (6), the *production* phase p on resource l expressed by $a_{pl} q_{pls}$ is bounded by the binary changeover variable $y_{p\prime pls}$ and a big-M factor C_{max}. This factor is equal to the length of a macroperiod to enable producing for a full macroperiod if the resource is set up for product p. The enforce setup constraint is imposed on all macroperiods.

$$\sum_{s \in S_t} a_{pl} q_{pls} \le \sum_{p' \in \mathbb{P}} y_{p\prime pls} C_{max} \qquad \forall p \in \mathbb{P}, l \in \mathbb{L}, t \in T \qquad (6)$$

Consistent changeover constraint. To relate changeover variables of two subsequent microperiods, a consistent changeover constraint is defined in Eq. (7). The changeover *to* a product p in microperiod $s-1$ must imply the changeover *from* the same product p in the next microperiod s on a resource l. Defining a transition product p' between two products p_1, p_2 of subsequent microperiods rather connecting products directly has shown a better computational performance during the model development. The consistent changeover constraint is imposed on all micro- and macroperiods.

$$\sum_{p_1 \in \mathbb{P}} y_{p_1 p\prime ls-1} = \sum_{p_2 \in \mathbb{P}} y_{p\prime p_2 ls} \qquad \forall p\prime \in \mathbb{P}, l \in \mathbb{L}, s \in S_t, t \in T \qquad (7)$$

Off-Shift constraint. No production or changeover is possible without operator personnel which is modeled by a shift schedule. A binary variable o_{lt} indicates whether there is no sufficient personnel in macroperiod t to operate resource l. As shown in Eq. (8), the duration of the *production* phase $a_{pl} q_{pls}$, as well as the *setup start* phase $h_{start,ls}$, and the *setup end* phase $h_{end,ls}$ is bounded by the indicator o_{lt} multiplied with the big-M factor C_{max} in all microperiods s of a macroperiod t. Consequently, if personnel does not suffice to operate resource l in a macroperiod, o_{lt} is equal to 1 and the duration of production and setup activities must be equal to 0. The off-shift constraint is imposed on all macroperiods.

$$h_{start,ls} + h_{end,ls} + \sum_{p \in \mathbb{P}} a_{pl} q_{pls} \le C_{max}(1 - o_{lt}) \qquad l \in \mathbb{L}, s \in S_t, t \in T \quad (8)$$

Microperiod constraint. We use microperiods to model 4 different production phases, in which a processing resource l can be. As shown in Eq. (9), the starting time k_{ls} of microperiod s on a resource l is enforced to be equal to the starting time of the previous microperiod k_{ls-1} plus the lengths of the *setup start* phase $h_{start,ls}$, the *production* phase $a_{pl} q_{pls}$, the *idle* phase $h_{idle,ls}$ and the *setup end* phase $h_{start,ls}$. The microperiod constraint is imposed on all processing resources, microperiods and macroperiods.

$$k_{ls} = k_{ls-1} + h_{start,ls} + \sum_{p \in \mathbb{P}} a_{pl} q_{pls} + h_{idle,ls} + h_{end,ls} \qquad \forall l \in \mathbb{L}, s \in S_t, t \in T \qquad (9)$$

Setup split constraint. In order to flexibly model the product-dependent changeovers, the changeover times $ct_{pp\prime l}$ can be split into a first part that takes place in the *setup end* phase of microperiod $s-1$ and a second part that takes place in the *setup start* phase of the subsequent microperiod s as shown in Eq. (10). Due to the variable lengths of the setup phases, a changeover time can occupy two full, subsequent microperiods, and consequently two full macroperiods if required. If the changeover time can be realized within $h_{end,ls-1}$, the subsequent *setup start* phase $h_{start,ls}$ takes on a value of 0. The setup split constraint is imposed on all processing resources, microperiods and macroperiods.

$$h_{end,ls-1} + h_{start,ls} = \sum_{p,p\prime \in \mathbb{P}} y_{pp\prime ls} ct_{pp\prime l} \qquad \forall l \in \mathbb{L}, s \in S_t, t \in T \qquad (10)$$

Micro-macro connector constraint. The start time of every first microperiod in a macroperiod must be equal to the start time of the tth macroperiod, where C_{max} denotes the fixed length of a macroperiod. As shown in Eq. (11) the micro-macro connector constraint is imposed on all processing resources and macroperiods.

$$k_{l,s=1} = (t-1) \cdot C_{max} \qquad \forall l \in \mathbb{L}, t \in T \qquad (11)$$

Personnel constraint. As shown in Eq. (12), the maximum number of processing resources in processing stage i that can be operated simultaneously in a macroperiod t is limited by the overall staffing level $F^i_{max,t}$. This parameter allows to model shift schedules for each processing stage i with a time granularity of macroperiods. In practice, shifts often do not overlap and the staffing level is constant within a shift. In this case, the length of a macroperiod can be chosen as the length of a shift. Otherwise, the length of a macroperiod must be chosen smaller to be able to model the staffing level accurately. The term $|\mathbb{L}_i|$ denotes the number of processing resources in stage i, while the term $\sum_{l \in \mathbb{L}_i} o_{lt}$ denotes the number of processing resources in stage i that are *not* staffed with personnel in macroperiod t. Consequently, the term $|\mathbb{L}_i| - \sum_{l \in \mathbb{L}_i} o_{lt}$ represents the number of processing resources that are staffed and ready-to-operate as expressed by Eq. (8). The personnel constraint is imposed on all macroperiods.

$$|\mathbb{L}_i| - \sum_{l \in \mathbb{L}_i} o_{lt} \le F^i_{max,t} \qquad with \quad i = 1, 2 \qquad \forall t \in T \qquad (12)$$

Maximum inventory constraint. As shown in Eq. (13), the inventory of intermediate product I_p is limited by a maximum inventory parameter I^{max}, which represents the total buffer capacity of all buffer tanks. If $I^{max} = 0$ quantities of intermediate that are produced in a macroperiod t have to be finalized in the subsequent macroperiod. With $I^{max} > 0$ a limited quantity can be carried over as inventory between the macroperiods. The maximum inventory constraint is imposed on all macroperiods $t \in T$.

$$\sum_{p \in \mathbb{IP}} I_{pt} \leq I^{max} \qquad \forall t \in T \tag{13}$$

Minimum lot size constraint. The lot size for intermediate products must be greater or equal to the minimum batch-size on the processing resource. Since the minimum lot size still might take longer to produce than the length of one macroperiod, a fixed number of λ microperiods, each of which can occupy a full macroperiod, is assumed. However the minimum lot size must be realized within the total time horizon and $s+\lambda \leq |T|$. As shown in Eq. (14), the quantity of product p on resource l in microperiods s to $s+\lambda$ must be greater than the minimum lot size $q_{min,l}$, if changeover from another product $p\prime$ to product p took place in s. The minimum lot size constraint is imposed on all resources $l \in \mathbb{L}_1$, intermediate products $p \in \mathbb{IP}$, microperiods, and macroperiods.

$$\sum_{v=s}^{s+\lambda} q_{plv} \geq \sum_{\substack{p\prime \in \mathbb{IP} \\ p\prime \neq p}} y_{p\prime pls} q_{min,l} \qquad \forall p \in \mathbb{IP},\, l \in \mathbb{L}_1,\, s \in S_t,\, t \in T \tag{14}$$

Maximum shelf life constraint. A maximum shelf life constraint is specified in Eq. (15), which enforces the limited shelf life of agro-chemicals in production. Inventory I_{pt} of an intermediate product p in macroperiod t is limited by the production of associated finished product quantities in a fixed number of γ subsequent macroperiods. For the choice of γ, $s+\lambda \leq |T|$ must hold. The maximum shelf life constraint is imposed on all intermediate products $p \in \mathbb{IP}$ and macroperiods.

$$I_{pt} \leq \sum_{v=t}^{t+\gamma} \sum_{s \in S_v} \sum_{l \in \mathbb{L}_2} \sum_{\hat{p} \in \mathbb{FP}} b_{p\hat{p}} q_{\hat{p}ls} \qquad \forall p \in \mathbb{IP},\, t \in T \tag{15}$$

Additional constraints. All backlog variables $B_{\hat{p}t}$ must be greater or equal to 0 as shown in Eq. (16). This ensures that only positive backlog (deficit quantity) is propagated from one macroperiod to the next and that surplus quantity can only be created by building up inventory.

$$B_{\hat{p}t} \geq 0 \qquad \forall \hat{p} \in \mathbb{FP},\, t \in T \tag{16}$$

Backlog quantities of all products $\hat{p} \in \mathbb{FP}$ are allow to build up to a maximum $B_{\hat{p},max}$ as shown in Eq. (17). Backlog quantities can be prevented entirely by setting $B_{\hat{p},max} = 0$. This constraint is enforced in the second optimization step.

$$\sum_{t \in T} \sum_{\hat{p} \in \mathbb{FP}} B_{\hat{p}t} \leq B_{\hat{p},max} \tag{17}$$

To initialize inventories and backlogs, a microperiod $s = 0$ is defined. Since the setup split constraint (10) is enforced for all microperiods including the initialization microperiod, an additional constraint is required to ensure that no setup activities can take place in $s = 0$ as shown in Eq. (18). This similarly applies to the backlog variables $B_{\hat{p}0}$ as shown in Eq. (19). The initialization constraints are imposed in the first macroperiod $t = 1$, and for all resources l.

$$h_{end,l0} = 0 \qquad with \quad t = 1 \qquad \forall l \in \mathbb{L} \tag{18}$$

$$B_{\hat{p}0} = 0 \qquad with \quad t = 1 \qquad \forall \hat{p} \in \mathbb{FP} \tag{19}$$

4. Results

Time and computational resources often are limiting factors for industrial applications of optimization models. Therefore, we investigate the scalability of the time-bucket model with respect to (1) solution time, (2) convergence of bounds, and (3) solution quality. We consider the following problem size parameters.

1. We vary the number of processing resources in each stage to analyze the influence of more complex production systems.
2. We vary the number of macroperiods to analyze the influence of optimizing longer production periods.
3. We vary the number of microperiods per macroperiod to analyze the influence of a finer time structure within a macroperiod, which allows for more production changeovers within a macroperiod.
4. We vary the number of products to analyze the influence of a fragmented production demand and production changeovers.

In addition, it is important to assess variability of (1) and (2) when solving models with the same size parameters but different input parameter sets, for instance, different production demand sets, production coefficients or shift schedules. Therefore we solve a set of 50 randomly generated instances for each model configuration. To generate the instances, we sample the following parameters from uniform distributions.

1. We vary the production demand $D_{\hat{p}t}$, which contains a subset of 25% of all finished products $\hat{p} \in \mathbb{FP}$. First, we compute a conservative estimate of the total production capacity. For that, we multiply the minimum run rate for each production stage with the number of resources per stage, and take the minimum capacity of all stages. Second, we assume that 30% of the products are high runners, which occupy 50% of the total production capacity equally. The other products are low runners, which occupy the remaining capacity equally.
2. We vary the changeover times $ct_{pp\prime l}$ for all products $p \in \mathbb{P}$ and resources $l \in \mathbb{L}$. We take a uniform sample from $[2, 16]$ hours.
3. We vary the production coefficients a_{pl} of all products $p \in \mathbb{P}$ and for all resources $l \in \mathbb{L}$. For the first stage we take a uniform sample a_{pl} from $[1.5, 15]\,\mathrm{h/volumetric\,unit}$ and for the second stage from $[0.5, 10]\,\mathrm{h/volumetric\,unit}$.
4. We vary the staffing levels $F^i_{max,t}$. We assume that all production stages are staffed with 70% on average.
5. We vary the minimum lot-size $q_{min,l}$ for all stage 1 processing resources $l \in \mathbb{L}_1$. We take a uniform sample from $[5, 20]$ volumetric units.

Furthermore we set the following parameters as fixed.

1. We fix the bill of material coefficients $b_{p\hat{p}}$ such that each intermediate product p can be converted into 3 finished products $\hat{p}$.
2. We fix C_{max} to 8 hours, which equals the length of one shift.
3. We fix I^{max}_p to 275 volumetric units, which is limiting the total quantity of all intermediate products stored as inventory $\sum_{p \in \mathbb{IP}} I_{pt}$ between the stages. This value corresponds to the sum of all buffer tank capacities.
4. We fix γ to 6, which sets the maximum number of microperiods in which quantities must be unloaded from inventory.
5. We fix $B_{\hat{p},max}$ to 0, which limits the maximum backlog quantity of finished product $\hat{p}$.
6. We fix the number of microperiods in which the minimum lot size must be realized to 2.

4.1. Solution time

Long solution times of MILP models often are prohibitive in the context of real-world applications. Therefore we analyze the solution time of the proposed model formulation by solving randomized instances and scaling up the problem size with respect to the number of processing resources, micro- and macroperiods as well as products. The different model configurations are shown in Table 2. We denote that with 1 microperiod per macroperiod we obtain a time grid in which each macroperiod still contains 4 flexible phases.

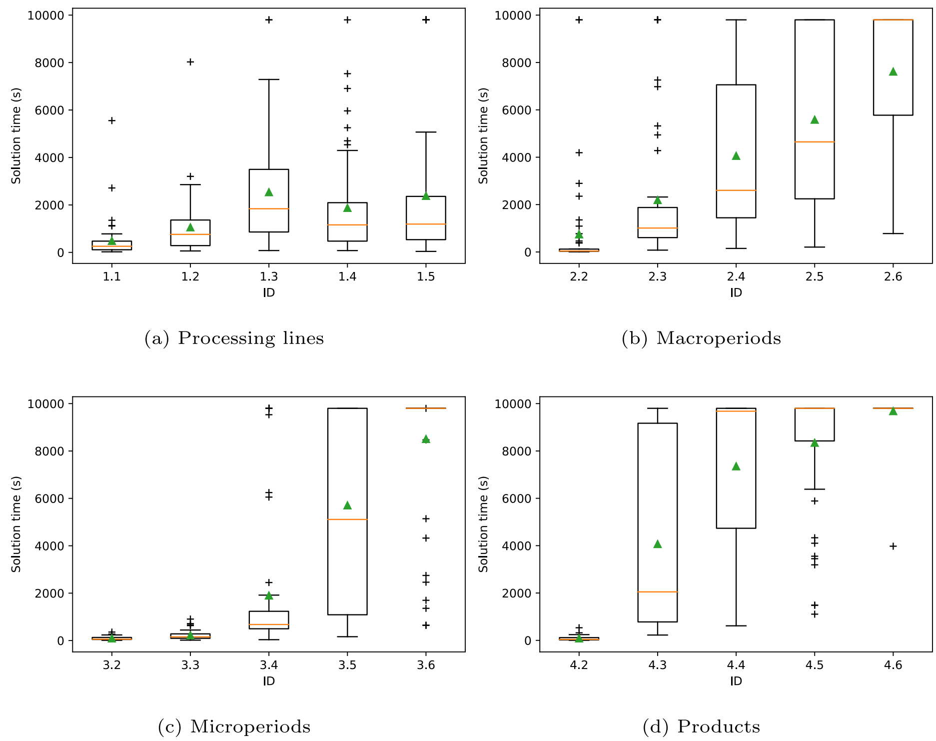


Fig. 5. Solution time distributions of model configurations with different (a) number of processing lines, (b) number of macroperiods, (c) number of microperiods per macroperiod, (d) number of products with median (orange line) and mean (green triangle) solution time. Solution time of unsolved instances set to 9800 s.

Table 2
Model overview.

ID	Proc res	Macropds	Micropds	Products	Unsolved[a,c]	Gap[b,c]
1.1	5 × 5	30	1	10 × 30	0	–
1.2	6 × 6	30	1	10 × 30	0	–
1.3	7 × 7	30	1	10 × 30	4.1	5.3
1.4	8 × 8	30	1	10 × 30	2.0	12.8
1.5	10 × 10	30	1	10 × 30	14.3	19.2
2.2	5 × 5	15	1	10 × 30	4.3	12.6
2.3	5 × 5	45	1	10 × 30	8.5	5.3
2.4	5 × 5	60	1	10 × 30	21.3	12.4
2.5	5 × 5	75	1	10 × 30	36.2	16.8
2.6	5 × 5	90	1	10 × 30	66.0	18.0
3.2	5 × 5	30	2	10 × 30	0	–
3.3	5 × 5	30	3	10 × 30	0	–
3.4	5 × 5	30	5	10 × 30	8.5	14.6
3.5	5 × 5	30	7	10 × 30	49.0	16.3
3.6	5 × 5	30	9	10 × 30	78.7	33.0
3.7	3 × 3	6	2	10 × 30	0	–
3.8	3 × 3	6	3	10 × 30	0	–
3.9	3 × 3	6	4	10 × 30	0	–
3.10	3 × 3	6	5	10 × 30	0	–
4.2	5 × 5	30	1	8 × 24	0	–
4.3	5 × 5	30	1	13 × 39	24.0	7.4
4.4	5 × 5	30	1	15 × 45	50.0	9.6
4.5	5 × 5	30	1	17 × 51	65.3	10.7
4.6	5 × 5	30	1	20 × 60	98.0	18.3

[a]Percent of unsolved instances within a solution time of 9800 s per instance.
[b]Average remaining optimality gap of unsolved instances at time out.
[c]Using Gurobi 9.5.2 on a CPU with 16 cores 3.4 GHz, 64 GB RAM.

Fig. 5 shows the solution time distributions of model configurations with different (a) number of processing lines, (b) number of macroperiods, (c) number of microperiods per macroperiod, and (d) number of products. We find that the solution time increases sharply as the size of the problem increases with respect to real world parameters such as the number of processing lines and products, as well time-bucket parameters such as the number of macro- and microperiods. From the high variability of solution times, we conclude that for complex models, computational effort can be strongly influenced by input parameter sets such as the specific production demand and shift schedules.

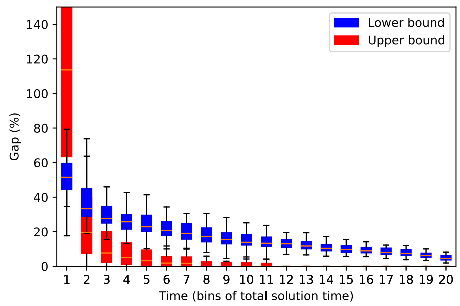
4.2. Bound convergence

A well-known drawback of time-bucket models is a weak LP relaxation due to the many binary variables and big-M formulations. Therefore, we extend our analysis to the evolution of the upper and lower bounds. In particular, we compute the remaining optimality gaps for upper and lower bound as shown in Eqs. (20) and (21). The main idea behind this is to analyze how upper and lower gaps converge to 0 separately. While the remaining gap of the upper bound Gap_{UB} provides information on the incumbent solution quality, the remaining gap of the lower bound Gap_{LB} provides information on the potential improvement of the incumbent solution. This information may ultimately be used to justify a truncated MIP search.

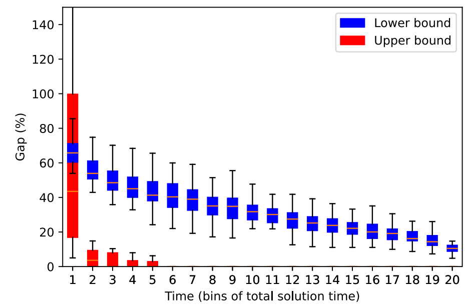
$$Gap_{UB} = \frac{UB_{Current} - Opt}{Opt} \tag{20}$$

$$Gap_{LB} = \frac{Opt - LB_{Current}}{Opt} \tag{21}$$

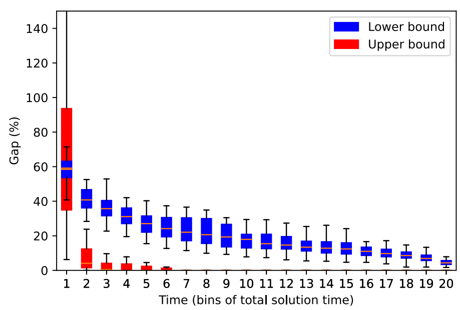
We perform solution time normalization and binning in order to compare instances with different absolute solution times. For that, we first normalize absolute solution times using the total solution times from our previous analysis in Section 4.1. Next we define 20 equal-widths intervals, each covering 5% of normalized solution time. Thereafter, we compute the representative average for upper and lower bounds within each interval based on all recorded values in that interval. The



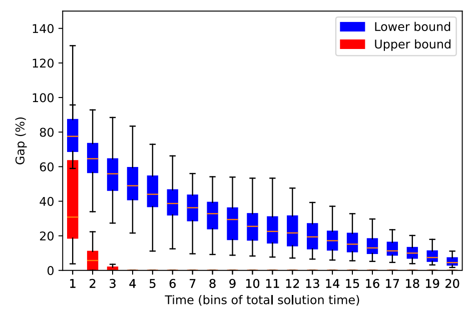
(a) ID 1.1: 5x5 processing lines



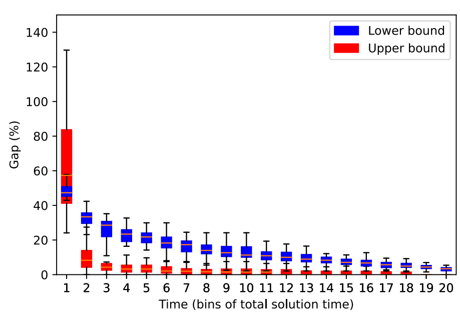
(b) ID 1.5: 10x10 processing lines



(c) ID 2.6: 75 macroperiods



(d) ID 3.4: 5 microperiods per macroperiod



(e) ID 4.4: 15 unpackaged products, 45 packaged products

Fig. 6. Evolution of optimality gaps of upper and lower bound for different model configurations. The gap values were averaged within 20 intervals each covering 5% of the normalized solution time.

evolution of upper and lower bounds for 5 different model configurations is presented in Fig. 6. We increase the number of processing lines in model 1.5, the number of macroperiods in model 2.6, the number of microperiods per macroperiod in model 3.4 and the number of products in model 4.4, and compare these models to the baseline model 1.1.

As shown in Fig. 6 upper bounds quickly converge to the optimum, while lower bounds slowly converge to the optimum. We observe that this effect becomes more pronounced for increasing problem sizes in all 4 size dimensions. First, we conclude that lower bounds of the time-bucket model generally become weaker when increasing the problem size in with respect to each of the 4 size parameters. This leads to slow convergence of the optimality gap, which eventually gives rise to long absolute solution times. Secondly, we denote that strong upper bounds are found early in the solution process despite of increasing problem size for all 4 parameters. Consequently, we are likely to obtain near optimal solutions with the time-bucket model when terminating the solution process prematurely.

4.3. Solution quality

Lastly, we study how the number of microperiods per macroperiod affects solution quality. We solve all random instances to optimality and compare the optimal changeover costs of model configuration 3.8, 3.9 and 3.10 to the costs of model configuration 3.7. As shown in Fig. 7, up to 17% lower changeover costs can be found when using more microperiods per macroperiod. More microperiods allow for more changeovers which can be beneficial if the triangle inequality for changeovers does not hold true. This situation can occur in chemical plants where some products have cleansing effect and can be used to shorten changeover times. In Fig. 7 we also observe similar solutions with 3 and 4 microperiods. This can be explained by minimum lot sizes and production rates, which limit the possible total number of changeovers. In addition, we denote that a sufficient number of microperiods must be defined to ensure that all products in demand can be scheduled at all. If this is not the case, the optimal total backlog

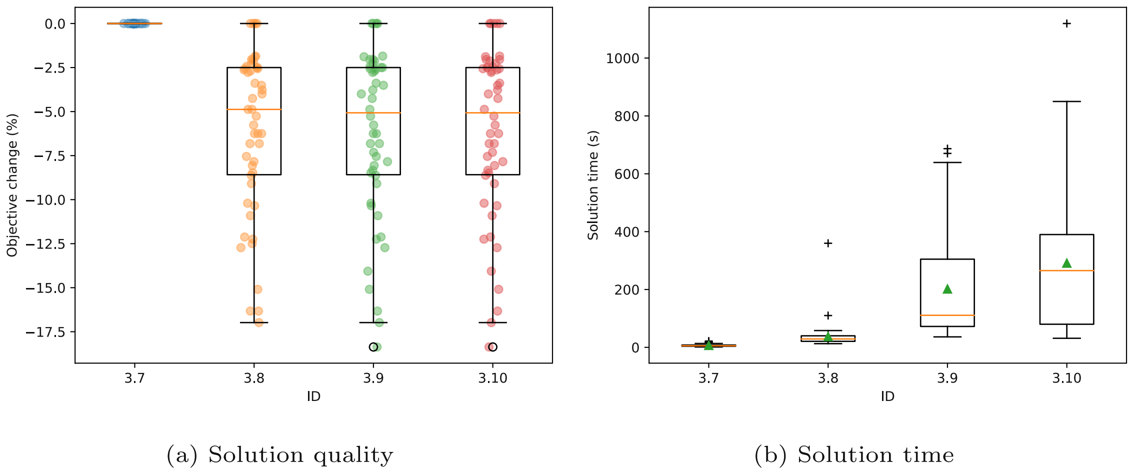


Fig. 7. Percentage change in objective value when increasing microperiods from 1 to 4, and solution time distribution. For each model configuration 50 instances were solved to optimality.

calculated in the first optimization step could be greater than 0. We conclude that depending on problem-specific parameters, increasing the number of microperiods per macroperiod can yield better solutions in both the first and second optimization step.

5. Case study

We consider the scheduling problem of a flexible flow shop in an industrial manufacturing plant for crop protection chemicals. The problem originates from the last two stages in the manufacturing process of agrochemicals, which are also known as product formulation and filling. The formulation and filling process takes place in a multi-product batch plant with 2 stages. In the first stage mixing, milling and reactions of raw materials take place, which results in intermediate products. In the second stage, the intermediate products are filled into final containers. The plant consists of multiple redundant, but not identical production lines per stage each capable of processing groups of agrochemical products. Because the formulation and filling process is the last station in the product supply chain, the process is exposed to a large number of raw materials at the input, and a highly fragmented demand of finished products at the output. Therefore, the production lines are designed for a high throughput of a broad variety of products, which results in a complex flow shop optimization problem.

5.1. Plant setup

A schematic overview of the process is shown in Fig. 8. Raw materials are mixed and processed in a first stage (formulation), which takes place in 7 redundant formulation lines $l \in \mathbb{L}_{form}$ and results in 50 different unpackaged products $p \in \mathbb{UP}$. In the second stage (filling), which takes place in 7 redundant filling lines $\hat{l} \in \mathbb{L}_{fill}$, the unpackaged products are filled into the final container, which results in 83 different packaged products $\hat{p} \in \mathbb{FP}$. We assume product- and line-specific changeover costs, and minimum lot sizes. The changeover matrices are not symmetrical, as the cleaning and changeover effort also depends on the product sequence. The set of both formulation and filling lines is denoted $\mathbb{L}$ and the set of both unpackaged and packaged products is denoted $\mathbb{P}$. There are 7 optional buffer tanks to decouple the two stages and maximize their utilization. They are modeled as one capacitated reservoir by the maximum inventory constraint in Eq. (13) and the maximum shelf life constraint in Eq. (15). The connectivity between lines and buffer tanks is not restricted. We consider different shift schedules for the formulation and the filling stage. The shift schedules determine the maximum number of lines that can be in the production or set-up phase at the same time due to the availability of operators. The bottleneck of the process varies with production demand and the shift schedules.

We optimize the formulation and filling process for a 1 month production period. Shift schedules are based on three 8 h shifts per day. Therefore we choose the length of a macroperiod to be equal to 8 h. Since no more than one production cycle can be realized within 8 h we choose 1 microperiod per macroperiod. The model specifications are summarized in Table 3 .

Table 3
Model specification.

Dimension/Feature	Modeled as
Time	30 days[a] as 90 macroperiods with 1 microperiod each
Unpackaged products	50 intermediate products
Packaged products	83 finished products
Formulation lines	7 processing resources as stage 1
Filling lines	7 processing resources as stage 2
Buffer tanks	1 capacitated reservoir
Changeovers	Product-sequence- and resource-dependent
Production rates	Product- and resource-dependent
Product conversion	Bill of material data gives conversion options
Product demand	Quantities of finished products with individual due dates
Operator resources	2 different shift schedules for stage 1 and 2
Minimum lot size	Product- and resource-dependent, only for stage 1

[a]We assume a production horizon of 30 days in the MILP model and 31 days in the DES model, since the DES model takes into account material transfer times between the tanks and logistics at the plant.

To describe formulation and filling process with our modeling approach, we make the following 2 assumptions.

1. Each formulation line and filling line is assumed to be one allocable processing resource. In the real-world plant, processing lines each consist of multiple machines, which are not relevant for modeling our optimization objective.
2. The buffer tanks are considered as one capacitated reservoir. As shown in the model constraints in Section 3.4 products can be loaded into the buffer system and unloaded (1) obeying a maximum shelf life constraint as shown in Eq. (15), and (2) up to a maximum reservoir capacity as shown in Eq. (13). An example inventory log for the capacitated reservoir can be found in Fig. A.1.

5.2. Results

First, we discuss the solution time and the evolution of the bounds. For that, we solve 5 different demands, of which 1 is the historic, original demand data set and 4 are alternative demand scenarios. Secondly,

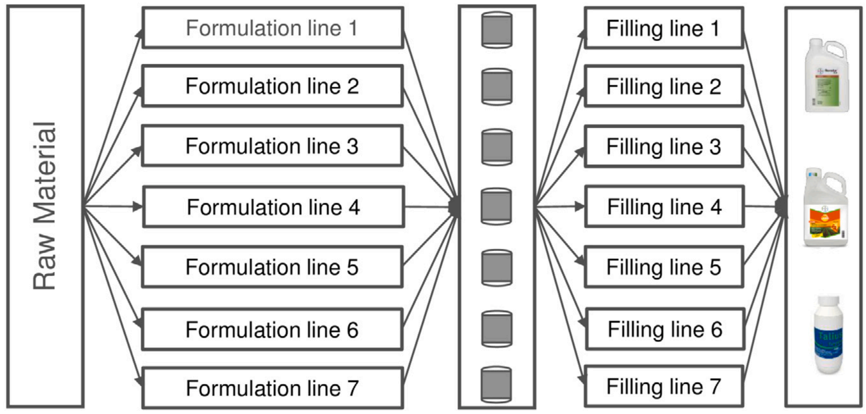
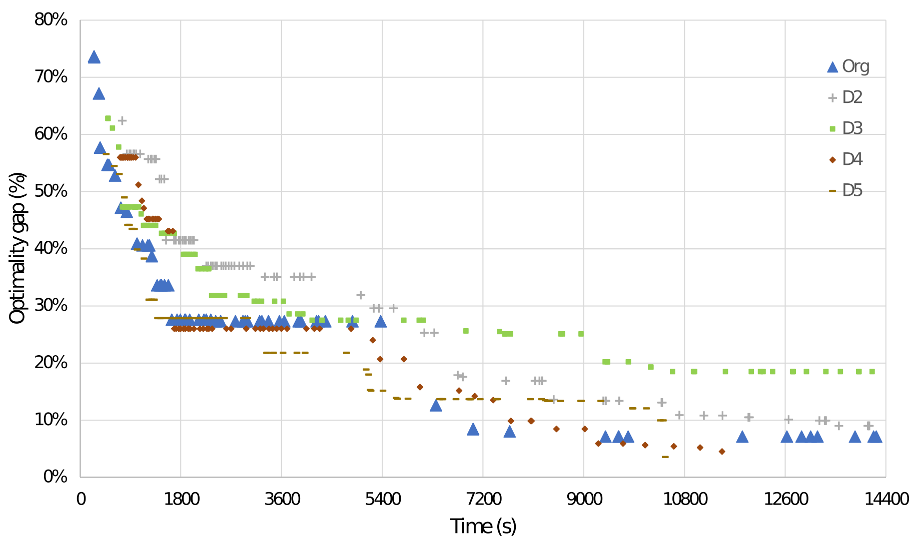
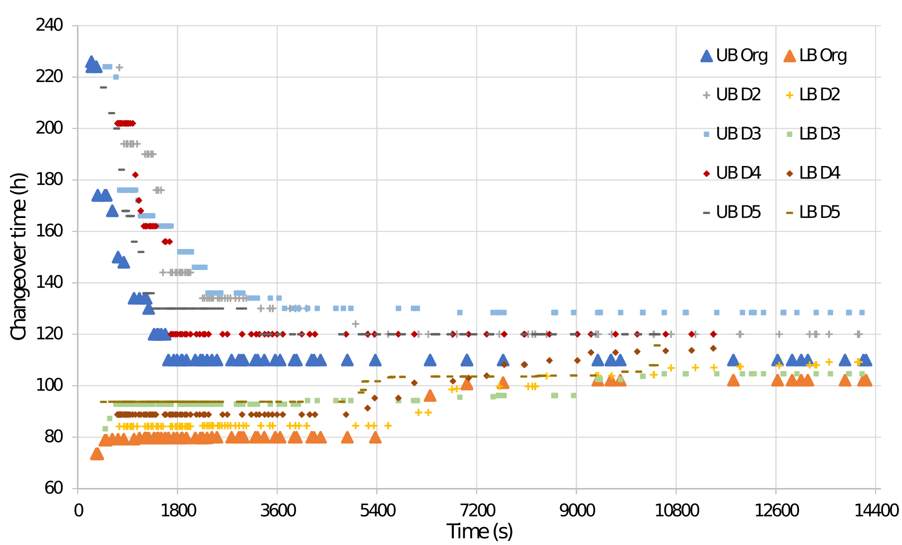


Fig. 8. Process overview: 7 formulation lines produce 50 unpackaged products, which can be stored in 7 buffer tanks and are consumed by 7 filling lines to produce 83 packaged products.



(a) Gaps



(b) Bounds

Fig. 9. Evolution of the remaining gaps (%) and bounds for different production demands for a solution phase of 4 h.

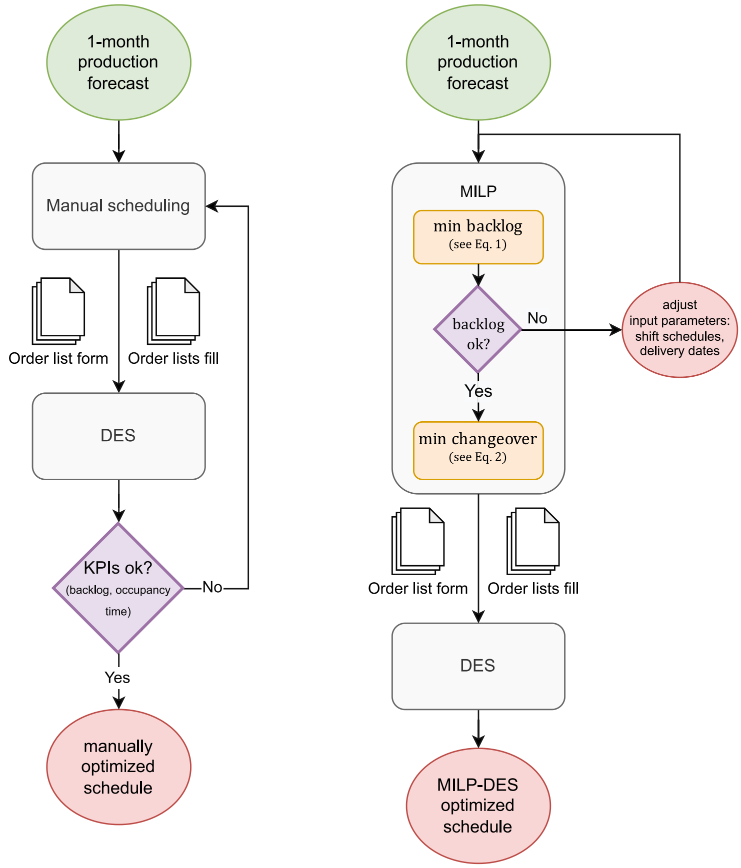


Fig. 10. Schematic overview of the manual scheduling workflow (left) and MILP scheduling workflow (right). Example order lists in Tables A.1, A.2.

we compare the MILP-optimized schedule with the manually optimized schedule of the historic demand data set. For that, we reconcile the MILP results with a validated DES model of the process. The DES model assigns production quantities to the 7 buffer tanks based on heuristics. We compare the MILP-DES schedule to the manually optimized DES schedule with respect to production backlog and occupancy time of the processing lines.

5.2.1. MILP solution

For the historic demand data set, we find a solution with no production backlog and 110 h of changeover time with a remaining gap of 27.3% after a total solution time of 1.22 h as further specified in Table 4. Optimization step 1 shows that the 1-month production demand $D_{\hat{p}t}$ can be satisfied without backlog in a makespan less than 31 days after 805 s solution time. Consequently a no-backlog constraint $\sum B_{\hat{p}t} = 0$ is enforced in the second optimization step, which minimizes the total changeover time to a value of 110 h after 3600 s solution time. For the alternative demand scenarios we observe similar results. Since the optimality gap is greater than 0 for all instances, we investigate the evolution of bounds and gap in the second optimization step over the course of 4 h as shown in Figs. 9(b) and 9(a).

As shown in Fig. 9, the remaining gap is decreasing further for all instances after 3600 s due to the improvement of the lower bounds. Near-optimal solutions are found relatively quickly which is a similar observation as in Section 4.2. Consequently, the solution phase can be terminated prematurely despite relatively large remaining gaps. We conclude that with the proposed model formulation near optimal solutions can be computed efficiently, but a proof of optimality is costly due to weak lower bounds.

Table 4
MILP results for a historic, original 1-month demand data set and 4 additional demand scenarios.

Set	Bcklg qty (%)	Chgovr (h)[a]	Gap (%)[b]	1st (s)[c,d]	2nd (s)[c,d]
Org	0	110	27.3	805	3600
Dmnd 2	0	130	35.1	659	3600
Dmnd 3	0	134	38.8	1033	3600
Dmnd 4	0	120	26.0	739	3600
Dmnd 5	0	120	21.8	828	3600

[a] In 2. stage gap after 1 h solution time.
[b] Remaining 2. stage gap after 1 h solution time.
[c] 1st stage objective shown in Eq. (1), second stage objective shown in Eq. (2).
[d] Using Gurobi 9.5.0 on a CPU with 16 cores 3.4 GHz, 64 GB RAM.

5.2.2. DES solution

The 2-step MILP optimization allows to adjust input parameters, such as sufficient staffing, shift schedules, and delivery dates for the demand, to ensure acceptable backlog and minimal changeover costs. The result of this MILP procedure is an optimized list of all production orders (campaign list) for the formulation and filling lines with start date, product type, lot size and line allocation. Example campaign lists are shown in Tables A.1 and A.2. Additionally, operator shift schedules can be computed based on the *set-up* and *production* phases of the allocated lines. For validation the campaign lists are reconciled using a validated DES model. Since the DES model is a high-fidelity model of the process the MILP results are rendered into an actionable production schedule. We compare the resulting MILP-DES schedule with a manually optimized DES (manual-DES) schedule. To obtain

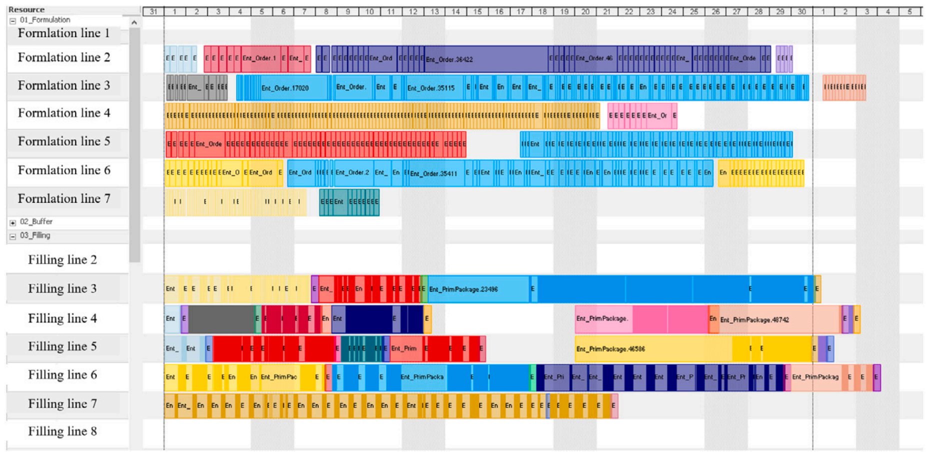


Fig. 11. Manually-optimized DES schedule of 7 formulation lines (top) and 7 filling lines (bottom), production orders are color-coded with respect to unpackaged products. Formulation line 1 and filling line 8 were not used in the original production data set.

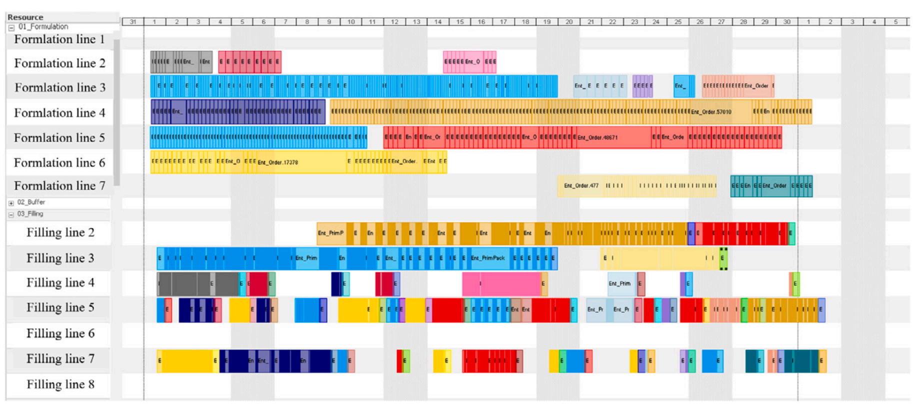


Fig. 12. MILP-optimized DES schedule of 7 formulation lines (top) and 7 filling lines (bottom), campaigns are color-coded with respect to unpackaged products. Formulation line 1 and filling line 8 were not used in the original production data set.

the latter, production planners generate campaign lists and refine them iteratively using the DES model. Both workflows are shown in Fig. 10.

From the makespans of the MILP-DES schedule and the manual-DES in Table 5, we conclude that the MILP approach is able to generate schedules that do not violate the delivery dates at the end of the month, while the manually optimized schedule contains backlog of approximately 2%. The adherence to delivery dates and demand quantities is ensured by minimizing the total backlog in the first optimization step (see Eq. (1)). When comparing the occupancy times of all lines in the formulation and filling stage, we observe that MILP-DES approach reduces the number of occupancy time by a total of 1218 machine hours. Approximately 10% formulation capacity and 27% filling capacity is freed as a result of minimizing the total changeover times in the second optimization step (see Eq. (2)). The additional capacity can be used to increase throughput, schedule maintenance intervals, but also to assess the robustness of the production schedule with regard to unplanned downtime, and spot demand. In Figs. 11 and 12, the manually optimized DES schedule and the MILP optimized DES schedule are shown. The Gantt charts show the allocation of formulation and filling lines by production campaigns. We observe the following differences:

1. Formulation lines

Table 5
MILP-DES results and manual-DES results for the reference month.

Method	Bcklg (% tot filled qty)	Mkspan (d)	Form (h)	Fill (h)
MILP-DES	0	31	3309	2251
manual-DES	2	34	3674	3104

1.1. There are 10 product changeovers on the formulation lines in the manual-DES schedule, and 9 in the MILP-DES schedule.

1.2. In the MILP-DES schedule, formulation campaigns are longer with little to no waiting times.

1.3. With the manual-DES schedule, the occupancy time of the formulation lines is higher than in the MILP-DES schedule. A lot of waiting time can be observed in the manual-DES schedule, for instance on formulation line 2 between day 13 and 18, on line 3 between day 4 and 18, and on line 6 between day 8 and 14.

1.4. In the manual-DES, schedule backlog is created by the last formulation campaign on line 3. It was not possible for scheduling experts to place this campaign manually into formulation and filling stage without backlog.

2. Filling lines

   2.1. There are 35 product changeovers on the filling lines in the manual-DES schedule, and 76 changeovers in the MILP-DES schedule.
   2.2. In the MILP-DES schedule, filling campaigns are short with little to no waiting time.
   2.3. In the manual-DES schedule, the occupancy time of the filling lines is higher than in the MILP-DES schedule. Much waiting time can be observed in the manual-DES schedule, for instance on filling line 5 between day 20 and 26, and on filling line 6 between day 18 and 28.
   2.4. In the MILP-DES schedule, packaged products coming from the same unpackaged product campaign (denoted by the same color), switch filling lines frequently. This is in contrast to the manual-DES schedule, in which long, uninterrupted filling campaigns are observed.

From observations (2.1), (2.2), (2.4), (1.3) and (1.4), we conclude that the MILP-DES approach uses a higher number changeovers on the filling lines to synchronize with the formulation stage. As a result of this synchronization, less changeover costs are incurred on the formulation lines (1.1) and no backlog is produced (see Table 5). A high number of changeovers on the filling lines also is justified by the fact that they are relatively inexpensive compared to formulation changeovers as less cleaning is required. Observation (1.4) illustrates the limits of manual scheduling based on operator experience and heuristics for complex problems. With the MILP-DES approach, a reduction of the total waiting times on all lines can be observed (1.2, 2.2). Table 5 shows that 365 machine hours are freed on all formulation lines and 853 h on all filling lines.

6. Conclusion

In this work, we developed a time-bucket MILP formulation for the lot-sizing and scheduling problem in a two-stage flow shop environment. The model applies two time grids, a microperiod and macroperiod time grid, which allow to include important real-world parameters such as lot-sizing, sequence dependent changeovers, buffer of intermediate bulk product, limited shelf life of products, and operator schedules. First, we investigated the time-bucket model with respect to solution time and bound convergence for different model configurations as well as randomized input parameters. Our analysis showed that near-optimal or optimal solutions can be found within moderate solution times of 1 h. Second, we demonstrated the applicability of the time-bucket formulation in an industrial case study of a 2-stage agrochemical production process, for which we proposed a 2-step solution procedure of the MILP model followed by a DES reconciliation step. We compared results of the MILP-DES approach with the results of a DES-aided, manual optimization approach, and observed that counterintuitive yet better schedules are found with respect to production backlog and resource utilization. We conclude that the time-bucket formulation represents viable industrial solution, that can be adopted for similar problems. Future work should go into the adoption of decomposition techniques to obtain stronger lower bounds.

CRediT authorship contribution statement

R. Wallrath: Investigation, Conceptualization, Data curation, Writing – original draft. **F. Seeanner:** Software (MILP model), Validation, Writing – review & editing. **M. Lampe:** Software (DES model), Validation. **M.B. Franke:** Conceptualization, Supervision, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

Acknowledgment

We thank the Bayer AG for providing the case study.

Appendix A. Attachments

The inventory log of the buffer tanks for an alternative demand scenario of the case study is shown in Fig. A.1. The maximum inventory constraint (see Eq. (13)) keeps the inventory level below 275 volumetric units. The DES model assigns intermediate product quantities to individual buffer tanks using an assignment rule. Quantities in Tables A.1, A.2 are given as rounded percentage of total production quantity. An example randomized model instance of model configuration ID1.1 can be found in the repository https://github.com/RoderickWR/time_bucket_MILP_formulation_for_optimal_lot_sizing_and_scheduling.

Table A.1
Example of a formulation order list from alternative demand scenario.

Order number	Line	Quantity (%)	Starting	Product ID
0	1	0.016	2020-06-02T14:00:00	Intermediate Product 1
1	1	0.013	2020-06-06T06:00:00	Intermediate Product 2
2	1	0.01	2020-06-09T22:00:00	Intermediate Product 3
3	2	0.004	2020-06-01T06:00:00	Intermediate Product 4
4	2	0.007	2020-06-01T18:00:00	Intermediate Product 5
5	2	0.006	2020-06-03T22:00:00	Intermediate Product 6
6	2	0.188	2020-06-04T22:00:00	Intermediate Product 4
7	2	0.012	2020-06-22T18:00:00	Intermediate Product 7
8	3	0.055	2020-06-01T06:00:00	Intermediate Product 8
9	3	0.166	2020-06-08T01:27:46	Intermediate Product 9
10	4	0.212	2020-06-01T06:00:00	Intermediate Product 4
11	4	0.133	2020-06-14T14:00:00	Intermediate Product 10
12	5	0.086	2020-06-04T14:00:00	Intermediate Product 11
13	6	0.072	2020-06-17T14:00:00	Intermediate Product 12
14	6	0.018	2020-06-25T06:00:00	Intermediate Product 13

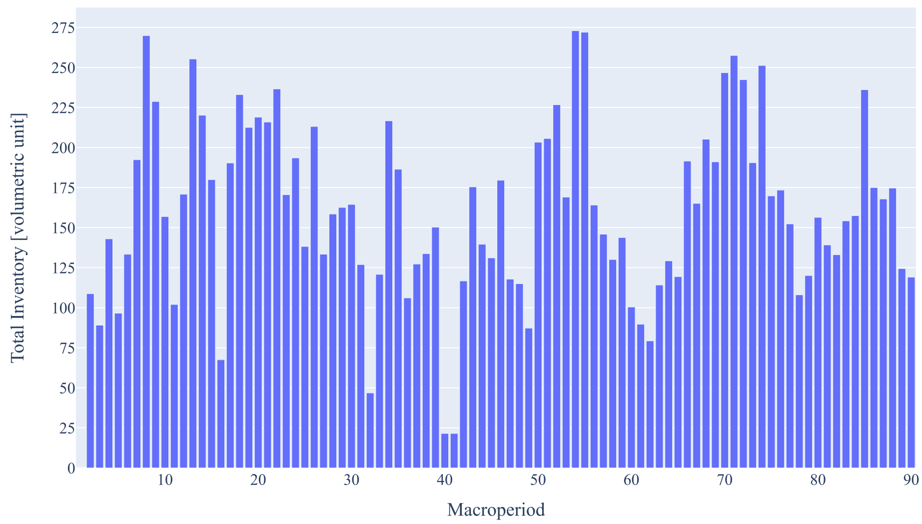


Fig. A.1. Inventory log of the capacitated reservoir.

Table A.2
Example of a filling order list from alternative demand scenario.

Order number	Line	Quantity (%)	Starting	Product ID
15	1	0.14	2020-06-08T22:00:00	Final Product 1
16	1	0.042	2020-06-27T14:00:00	Final Product 2
17	2	0.324	2020-06-01T14:00:00	Final Product 3
18	2	0.072	2020-06-19T06:00:00	Final Product 4
19	3	0.005	2020-06-01T14:00:00	Final Product 5
20	3	0.009	2020-06-03T06:00:00	Final Product 6
21	3	0.001	2020-06-04T06:00:00	Final Product 7
22	3	0.001	2020-06-04T22:00:00	Final Product 8
23	3	0.008	2020-06-05T14:00:00	Final Product 6
24	3	0.005	2020-06-06T14:00:00	Final Product 5
25	3	0.001	2020-06-10T06:00:00	Final Product 9
26	3	0.01	2020-06-11T06:00:00	Final Product 10
27	3	0.012	2020-06-23T06:00:00	Final Product 11
28	4	0.005	2020-06-02T06:00:00	Final Product 12
29	4	0.021	2020-06-03T14:00:00	Final Product 5
30	4	0.005	2020-06-05T06:00:00	Final Product 13
31	4	0.021	2020-06-05T22:00:00	Final Product 5
32	4	0.007	2020-06-09T14:00:00	Final Product 14
33	4	0.04	2020-06-10T06:00:00	Final Product 15
34	4	0.02	2020-06-15T14:00:00	Final Product 16
35	4	0.014	2020-06-17T06:00:00	Final Product 14
36	4	0.014	2020-06-18T22:00:00	Final Product 15
37	4	0.014	2020-06-19T22:00:00	Final Product 16
38	4	0.003	2020-06-21T06:00:00	Final Product 17
39	4	0.007	2020-06-23T14:00:00	Final Product 16
40	4	0.021	2020-06-24T06:00:00	Final Product 14
41	4	0.021	2020-06-25T14:00:00	Final Product 16
42	4	0.007	2020-06-26T22:00:00	Final Product 18
43	4	0.023	2020-06-28T14:00:00	Final Product 17
44	4	0.009	2020-06-30T14:00:00	Final Product 18
45	5	0.002	2020-06-01T22:00:00	Final Product 5
46	5	0.004	2020-06-02T14:00:00	Final Product 15
47	5	0.002	2020-06-03T06:00:00	Final Product 12
48	5	0.004	2020-06-05T06:00:00	Final Product 14
49	5	0.013	2020-06-08T06:00:00	Final Product 19
50	5	0.009	2020-06-12T06:00:00	Final Product 15
51	5	0.013	2020-06-17T14:00:00	Final Product 16
52	5	0.004	2020-06-18T22:00:00	Final Product 14
53	5	0.009	2020-06-19T14:00:00	Final Product 16
54	5	0.013	2020-06-20T14:00:00	Final Product 15
55	5	0.009	2020-06-22T22:00:00	Final Product 14
56	5	0.001	2020-06-25T14:00:00	Final Product 18
57	5	0.007	2020-06-26T06:00:00	Final Product 16
58	5	0.027	2020-06-29T06:00:00	Final Product 14

References

Basán, N.P., Cóccola, M.E., del Valle, A.G., Méndez, C.A., 2019. An efficient MILP-based decomposition strategy for solving large-scale scheduling problems in the offshore oil and gas industry. In: Kiss, A.A., Zondervan, E., Lakerveld, R., Özkan, L. (Eds.), 29th European Symposium on Computer Aided Process Engineering. In: Computer Aided Chemical Engineering, vol. 46, Elsevier, pp. 943–948. http://dx.doi.org/10.1016/B978-0-12-818634-3.50158-2, URL https://www.sciencedirect.com/science/article/pii/B9780128186343501582.

Berretta, R., França, P., Armentano, V., 2005. Metaheuristic approaches for the multilevel resource-constrained lot-sizing problem with setup and lead times. Asia Pac. J. Oper. Res. 22, 261–286.

Borisovsky, P., Eremeev, A., Kallrath, J., 2019. Multi-product continuous plant scheduling: combination of decomposition, genetic algorithm, and constructive heuristic. Int. J. Prod. Res. 58, 1–19. http://dx.doi.org/10.1080/00207543.2019.1630764.

Castro, P.M., 2022. Optimal scheduling of a multiproduct batch chemical plant with preemptive changeover tasks. Comput. Chem. Eng. 162, 107818. http://dx.doi.org/10.1016/j.compchemeng.2022.107818, URL https://www.sciencedirect.com/science/article/pii/S0098135422001569.

Castro, P., Aguirre, A., Zeballos, L., Méndez, C., 2011. Hybrid mathematical programming discrete-event simulation approach for large-scale scheduling problems. Ind. Eng. Chem. Res. 50, http://dx.doi.org/10.1021/ie200841a.

Castro, P.M., Grossmann, I.E., Zhang, Q., 2018. Expanding scope and computational challenges in process scheduling. Comput. Chem. Eng. 114, 14–42. http://dx.doi.org/10.1016/j.compchemeng.2018.01.020, FOCAPO/CPC 2017. URL https://www.sciencedirect.com/science/article/pii/S0098135418300449.

Clark, A., Morabito, R., Toso, E.A., 2011. Production setup-sequencing and lot-sizing at an animal nutrition plant through ATSP subtour elimination and patching. J. Sched. 14, 119. http://dx.doi.org/10.1007/s10951-009-0135-7.

Costa, A., 2015. Hybrid genetic optimization for solving the batch-scheduling problem in a pharmaceutical industry. Comput. Ind. Eng. 79, 130–147. http://dx.doi.org/10.1016/j.cie.2014.11.001, URL https://www.sciencedirect.com/science/article/pii/S0360835214003623.

Elekidis, A.P., Georgiadis, M.C., 2021. Production scheduling of flexible continuous make-and-pack processes with byproducts recycling. Int. J. Prod. Res. 1–23. http://dx.doi.org/10.1080/00207543.2021.1920058.

Elzakker, M., Zondervan, E., Raikar, N., Grossmann, I., Bongers, P., 2012. Scheduling in the FMCG industry: An industrial case study. Ind. Eng. Chem. Res. 51, 7800–7815. http://dx.doi.org/10.1021/ie202106k.

Floudas, C.A., Lin, X., 2004. Continuous-time versus discrete-time approaches for scheduling of chemical processes: a review. Comput. Chem. Eng. 28 (11), 2109–2129. http://dx.doi.org/10.1016/j.compchemeng.2004.05.002, URL https://www.sciencedirect.com/science/article/pii/S0098135404001401.

Frazzon, E.M., Albrecht, A., Hurtado, P.A., 2016. Simulation-based optimization for the integrated scheduling of production and logistic systems. IFAC-PapersOnLine 49 (12), 1050–1055. http://dx.doi.org/10.1016/j.ifacol.2016.07.581, 8th IFAC Conference on Manufacturing Modelling, Management and Control MIM 2016. URL https://www.sciencedirect.com/science/article/pii/S2405896316308394.

Georgiadis, G.P., Elekidis, A.P., Georgiadis, M.C., 2019. Optimization-based scheduling for the process industries: From theory to real-life industrial applications. Processes 7 (7), URL https://www.mdpi.com/2227-9717/7/7/438.

Georgiadis, G.P., Mariño Pampín, B., Adrián Cabo, D., Georgiadis, M.C., 2020. Optimal production scheduling of food process industries. Comput. Chem. Eng. 134, 106682. http://dx.doi.org/10.1016/j.compchemeng.2019.106682, URL https://www.sciencedirect.com/science/article/pii/S0098135419309603.

Gnoni, M., Iavagnilio, R., Mossa, G., Mummolo, G., Di Leva, A., 2003. Production planning of a multi-site manufacturing system by hybrid modelling: A case study from the automotive industry. Int. J. Prod. Econ. 85 (2), 251–262. http://dx.doi.org/10.1016/S0925-5273(03)00113-0, Supply Chain Management. URL https://www.sciencedirect.com/science/article/pii/S0925527303001130.

Harjunkoski, I., 2016. Deploying scheduling solutions in an industrial environment. Comput. Chem. Eng. 91, 127–135. http://dx.doi.org/10.1016/j.compchemeng.2016.03.029, 12th International Symposium on Process Systems Engineering & 25th European Symposium of Computer Aided Process Engineering (PSE-2015/ESCAPE-25), 31 May - 4 June 2015, Copenhagen, Denmark. URL https://www.sciencedirect.com/science/article/pii/S0098135416300916.

Klanke, C., Yfantis, V., Corominas, F., Engell, S., 2021. Short-term scheduling of make-and-pack processes in the consumer goods industry using discrete-time and precedence-based MILP models. Comput. Chem. Eng. 154, 107453. http://dx.doi.org/10.1016/j.compchemeng.2021.107453, URL https://www.sciencedirect.com/science/article/pii/S0098135421002313.

Kondili, E., Pantelides, C., Sargent, R., 1993. A general algorithm for short-term scheduling of batch operations—I. MILP formulation. Comput. Chem. Eng. 17 (2), 211–227. http://dx.doi.org/10.1016/0098-1354(93)80015-F, An International Journal of Computer Applications in Chemical Enginnering. URL https://www.sciencedirect.com/science/article/pii/009813549380015F.

Kopanos, G., Puigjaner, L., Georgiadis, M., 2011. Resource-constrained production planning in semicontinuous food industries. Comput. Chem. Eng. 35, 2929–2944. http://dx.doi.org/10.1016/j.compchemeng.2011.04.012.

Lee, H., Maravelias, C.T., 2018. Combining the advantages of discrete- and continuous-time scheduling models: Part 1. Framework and mathematical formulations. Comput. Chem. Eng. 116, 176–190. http://dx.doi.org/10.1016/j.compchemeng.2017.12.003, Multi-scale Systems Engineering – in memory & honor of Professor C.A. Floudas. URL https://www.sciencedirect.com/science/article/pii/S0098135417304337.

Maravelias, C., Grossmann, I., 2003. A new general continuous-time state task network formulation for short-term scheduling of multipurpose batch plants. Ind. Eng. Chem. Res. 42, 3056–3074. http://dx.doi.org/10.1021/ie020923y.

Méndez, C.A., Cerdá, J., Grossmann, I.E., Harjunkoski, I., Fahl, M., 2006. State-of-the-art review of optimization methods for short-term scheduling of batch processes. Comput. Chem. Eng. 30 (6), 913–946. http://dx.doi.org/10.1016/j.compchemeng.2006.02.008, URL https://www.sciencedirect.com/science/article/pii/S0098135406000287.

Meyr, H., 2004. Simultane Losgrößen- und Reihenfolgeplanung bei mehrstufiger kontinuierlicher Fertigung. Z. Betriebswirtschaft 74.

Nikolopoulou, A., Ierapetritou, M., 2012. Hybrid simulation based optimization approach for supply chain management. Comput. Chem. Eng. 47, 183–193. http://dx.doi.org/10.1016/j.compchemeng.2012.06.045.

Pantelides, C.C., 1994. Unified frameworks for optimal process planning and scheduling. In: Proceedings on the Second Conference on Foundations of Computer Aided Operations. pp. 253–274.

Pinedo, M., 2008. Scheduling: Theory, algorithms, and systems.

Qin, W., Zhuang, Z., Liu, Y., Tang, O., 2019. A two-stage ant colony algorithm for hybrid flow shop scheduling with lot sizing and calendar constraints in printed circuit board assembly. Comput. Ind. Eng. 138, 106115. http://dx.doi.org/10.1016/j.cie.2019.106115, URL https://www.sciencedirect.com/science/article/pii/S0360835219305844.

Sarin, S.C., Sherali, H.D., Liao, L., 2014. Primary pharmaceutical manufacturing scheduling problem. IIE Trans. 46 (12), 1298–1314. http://dx.doi.org/10.1080/0740817X.2014.882529.

Schilling, G., Pantelides, C., 1996. A simple continuous-time process scheduling formulation and a novel solution algorithm. Comput. Chem. Eng. 20, S1221–S1226. http://dx.doi.org/10.1016/0098-1354(96)00211-6, European Symposium on Computer Aided Process Engineering-6. URL https://www.sciencedirect.com/science/article/pii/0098135496002116.

Seeanner, F., Meyr, H., 2013. Multi-stage simultaneous lot-sizing and scheduling for flow line production. OR Spectrum 35, http://dx.doi.org/10.1007/s00291-012-0296-1.

Sel, C., Bilgen, B., Bloemhof-Ruwaard, J., van der Vorst, J., 2015. Multi-bucket optimization for integrated planning and scheduling in the perishable dairy supply chain. Comput. Chem. Eng. 77, 59–73. http://dx.doi.org/10.1016/j.compchemeng.2015.03.020, URL https://www.sciencedirect.com/science/article/pii/S0098135415000915.

Tempelmeier, H., Helber, S., 1994. A heuristic for dynamic multi-item multi-level capacitated lotsizing for general product structures. European J. Oper. Res. 75 (2), 296–311. http://dx.doi.org/10.1016/0377-2217(94)90076-0, URL https://www.sciencedirect.com/science/article/pii/0377221794900760.

Toledo, C.F.M., de Oliveira, R.R.R., Morelato França, P., 2013. A hybrid multi-population genetic algorithm applied to solve the multi-level capacitated lot sizing problem with backlogging. Comput. Oper. Res. 40 (4), 910–919. http://dx.doi.org/10.1016/j.cor.2012.11.002, URL https://www.sciencedirect.com/science/article/pii/S0305054812002341.

Wörbelauer, M., Meyr, H., Almada-Lobo, B., 2019. Simultaneous lotsizing and scheduling considering secondary resources: a general model, literature review and classification. OR Spectrum 41, http://dx.doi.org/10.1007/s00291-018-0536-0.

Wu, T., Akartunalı, K., Song, J., Shi, L., 2013. Mixed integer programming in production planning with backlogging and setup carryover: Modeling and algorithms. Discrete Event Dyn. Syst. 23, http://dx.doi.org/10.1007/s10626-012-0141-3.