# Continuous-Time Models for Short-Term Scheduling of Multipurpose Batch Plants: A Comparative Study 

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#### Abstract

During the last two decades, the problem of short-term scheduling of multiproduct and multipurpose batch plants has gained increasing attention in the academic, research, and manufacturing communities, predominantly because of the challenges and the high economic incentives. In the last 10 years, numerous formulations have been proposed in the literature based on continuous representations of time. The continuous-time formulations have proliferated because of their established advantages over discrete-time representations and in the quest to reduce the integrality gap and the resulting computational complexities. The various continuous-time models can be broadly classified into three distinct categories: slot-based, global event-based, and unit-specific event-based formulations. In this paper, we compare and evaluate the performance of six such models, based on our implementations using several benchmark example problems from the literature. Two different objective functions, maximization of profit and minimization of makespan, are considered, and the models are assessed with respect to different metrics such as the problem size (in terms of the number of binary variables, continuous variables, and constraints), computational times (on the same computer), and number of nodes needed to reach zero integrality gap. Two additional computational studies with resource constraints such as utility requirements are also considered.


## 1. Introduction

The problem of short-term scheduling of multiproduct and multipurpose batch plants has received significant attention from both academic and industrial researchers in the past few years, primarily

[^0]because of the challenges and the high economic tradeoffs involved. Recently, Floudas and Lin ${ }^{1,2}$ presented state-of-the-art reviews comparing various discrete and continuous time-based formulations. The different continuous-time models proposed in the literature can be broadly classified into three distinct categories: slot-based, global event-based, and unit-specific eventbased formulations.

One of the first methods used to formulate continuous-time models for the scheduling of network-represented or sequential processes is based on the concept of time slots. Time slots represent the time horizon in terms of ordered blocks of unknown, variable lengths, or slots, as presented by Pinto and Grossmann, ${ }^{3-6}$ Karimi and McDonald, ${ }^{7}$ Lamba and Karimi, ${ }^{8,9}$ and recently by Sundaramoorthy and Karimi. ${ }^{10}$ In addition, alternate methods have been developed which define continuous variables directly to represent the timings of tasks without the use of time slots. These methods, for both network-represented and sequential processes, can be classified into two different representations of time, global event-based models and unit-specific event-based models. Global event-based models use a set of events that are common across all units, and the event points are defined for either the beginning or end (or both) of each task in each unit. Research contributions following this direction include those presented by Zhang and Sargent, ${ }^{11,12}$ Mockus and Reklaitis, ${ }^{13-15}$ Schilling and Pantelides, ${ }^{16,}{ }^{17}$ Mendez and co-workers, ${ }^{18-20}$ Castro and coworkers., ${ }^{21,22}$ Mendez and Cerda, ${ }^{23}$ Majozi and Zhu, ${ }^{24}$ Lee et al., ${ }^{25}$ Burkard et al., ${ }^{26}$ Wang and Guignard, ${ }^{27}$ and Maravelias and Grossmann. ${ }^{28}$ Note that the concept of time slots has changed over a period of time. Earlier models were based on the assignment of tasks to time slots, while in the recent models, continuous variables are used to directly assign tasks to different time points; and hence, these are more similar to global event-based models. The only difference seems to be that the length of the common-time grid is referred to as the time slot explicitly in some slot-based formulations (for instance by Sundaramoorthy and Karimi ${ }^{10}$ ).

On the other hand, unit-specific event-based models, originally developed by Floudas and co-workers, ${ }^{29-36}$ define events on a unit basis, allowing tasks corresponding to the same event point but in different units to take place at different times. This representation is considered the most general, compact, and "true" continuous-time model (as is demonstrated later in this paper) used in short-term scheduling. Another unit-specific event-based continuous-time model was developed by Giannelos and Georgiadis. ${ }^{37}$ However, because of special sequencing restrictions of the same start and finish times on tasks consuming or producing the same state, it is effectively transformed into a global event-based model. Their formulation is similar to that by Ierapetritou and Floudas; ${ }^{29}$
however, because of the special sequencing constraints, their model leads to suboptimal solutions for batch plants as noted by Sundaramoorthy and Karimi ${ }^{10}$ and also as demonstrated later in this paper. Most of the above-mentioned formulations have been based on either state-task network (STN) or resource-task network (RTN) process representations, except the model of Sundaramoorthy and Karimi, ${ }^{10}$ which is based on generalized recipe diagrams.

The different time representations are summarized in Figure 1. In the uniform time discretization depicted in Figure 1a, the time horizon is divided into intervals of equal length that are common across all units.


Figure 1. Different time representations.

Parts b-d of Figure 1 illustrate the different variations in the continuous-time representations. In the slot-based continuous-time representation of Figure 1b, the time horizon is divided into time intervals of unequal and unknown lengths, and typically tasks need to start and finish at an event ( $n$ slots are equivalent to $n+1$ events). In the global event-based continuous-time representation of Figure 1c, only the start times of the tasks need to be at an event point and the events considered are common across all units. In the unit-specific event-based time representation of Figure 1d, only
the start time of each task in a unit has to be at an event point, whereas the occurrences of each event can be different across different units. For the specific instance of the four tasks considered on three units in parts b-d of Figure 1, the slot-based representation requires 5 slots (or 6 events), the global event-based representation requires 4 events, while the unit-specific event-based representation requires consideration of only 2 events. It should be noted that hybrid methods have also been developed ${ }^{38}$ which combine mixed-integer linear programming (MILP) models with constraint programming. These are not within the scope of the presented comparison, which aims at evaluating pure MILP approaches for the aforementioned classes.

In this paper, we compare the ability of closing the integrality gap and evaluate the performance of the above-mentioned short-term scheduling formulations based on our implementations of these models. Specifically, we compare the slot-based models (Sundaramoorthy and Karimi ${ }^{10}$ ) versus global event-based models (Maravelias and Grossmann ${ }^{28}$ and Castro and co-workers. ${ }^{21,22}$ ) versus the unit-specific event-based models (Ierapetritou and Floudas ${ }^{29}$ and Giannelos and Georgiadis ${ }^{37}$ ), and study the computational effectiveness of each. Both network-represented and sequential processes are considered along with two scheduling objectives: maximization of profit and minimization of makespan. We also introduce two computational studies that compare the models of Maravelias and Grossmann, ${ }^{28}$ Castro et al., ${ }^{22}$ and Janak et al. ${ }^{35}$ for resource constraints.

The rest of the paper is organized as follows. In Section 2, we describe the different performance metrics with which the above-mentioned models are compared. The formulations for the different models used for comparison in this study are briefly discussed in Section 3, followed by the illustration of the benchmark examples in Section 4. The computational results and discussion for problems without resource constraints are detailed in Section 5 followed by computational studies with resource constraints in Section 6. The implemented formulations for each model are summarized in the appendices.

## 2. Description of Performance Metrics

Numerous formulations proposed in the literature, often claiming superiority over each other, exist for short-term scheduling of batch plants using continuous-time representations. Hence, for a fair and legitimate comparison of the different models with respect to their computational effectiveness, the following metrics are defined:
(a) Benchmark examples: The examples chosen are standard benchmark examples from the recent literature, used by many of the researchers in short-term scheduling of multipurpose batch plants. Both the STN- and RTN-based process representations are considered with variable batch sizes and processing times. The resource constraints considered are only those related to the raw material and equipment availability in the first three examples. Resource constraints related to utility requirements are considered in examples 4 and 5. The various models are evaluated for multiple instances of each problem with different time horizons and demand distributions and with respect to two dissimilar objective functions, maximization of profit and minimization of makespan. The latter objective of makespan minimization is considered to be more rigorous for assessing the performance of different models, as most of the models proposed in the literature have difficulties in closing the integrality gaps for this case.
(b) Completion to global optimality: While solving an optimization problem, completion to optimality in order to close the integrality gap is important for a fair comparison of different models. Unlike some of the comparisons reported in the literature, in this paper, all the problems are solved to zero integrality gap, except in some cases when one or more models take excessive computational time to solve to the reported global optimal solution, compared to the other models. For each model and for each instance of the various examples, we study parametrically the increase of the number of events or slots until there is no further improvement in the objective function, as suggested by Ierapetritou \& Floudas ${ }^{29}$.
(c) Computer hardware and software: The computer hardware and software used for comparing different models also has a noteworthy influence on the computational time taken to solve to zero integrality gap (as is also noted recently by Sundaramoorthy and Karimi ${ }^{10}$ ). The performance of the same model would be different on computers with different hardware (speed, RAM, etc.). Also, the computational performance would be different with a different version of the optimization software used (for instance, different versions of GAMS and its solvers). Hence, for a valid comparison, all the models are implemented on the same computer ( 3 GHz Pentium 4 with 2 GB RAM) and under similar conditions (GAMS distribution 21.1, CPLEX 8.1.0). For the solvers, only the default option values are used.
(d) Model implementation: In contrast to most of the comparisons reported in the literature, in this paper, the various formulations are compared based on our own implementation of the abovementioned models. Before applying each model to the benchmark problems considered in this
paper, each of the models is first reproduced against the examples presented in the original paper, to match the reported model statistics (number of variables and constraints) as best as possible. Sometimes, the reported statistics do not match with our implementation, possibly because of the usage of additional constraints not reported in the relevant paper. The model formulations we implemented are reported in the appendices.
(e) Model statistics: The number of binary variables and constraints resulting from a model has a significant impact on its computational performance. The different models are compared with respect to the resulting number of binary variables, the total number of continuous variables and constraints used, the total number of nodes explored to reach zero integrality gap, the computational times (CPU seconds) on the same computer, the objective function value at the relaxed node, and the number of nonzero elements in the resulting coefficient matrix. Although the number of nodes explored does not depend on the computer hardware, is often found to be mildly dependent on the order in which the constraints are written, for instance, while implementing the models in GAMS. ${ }^{39}$ Also, the $M$ value used in the big-M constraints may affect the value of the objective function at the relaxed node, and also may affect the computational time. However, we used a common value of $M$ for all the models instead of exploring the best value of $M$ for each model that requires big-M constraints.

## 3. Descriptions of Different Continuous-Time Models for Batch Plants

Six different continuous-time models for batch plants are considered in this comparative study. They have been selected on the basis of representing all possible classes: slot-based, global eventbased, and unit-specific event-based models. Also, the papers of Castro and co-workers., ${ }^{21,22}$ Giannelos and Georgiadis, ${ }^{37}$ Maravelias and Grossmann, ${ }^{28}$ and Sundaramoorthy and Karimi ${ }^{10}$ each provided comparisons with other approaches. The key features and the differences among the various continuous-time models compared in this paper are briefly discussed below, in chronological order.
3.1. Unit-Specific Event-Based Model of Ierapetritou and Floudas ${ }^{29}$ (I\&F). The authors presented the original concept of event points which correspond to a sequence of time instances located along the time axis of each unit, each representing the beginning of a task or the utilization of the unit. The location of event points is different for each unit, allowing different tasks to start at
different times in each unit for the same event point. The timings of tasks are accounted through special sequencing constraints involving big-M constraints. No resources other than materials and equipment are considered. Although the model originally claimed its superiority due to both decoupling of task and unit events and nonuniform-time grid, later it became evident that it is primarily the introduction of the unit-specific events that gives the model the resulting cutting edge and makes it a class apart from all other models proposed in the literature. The resulting model requires less event points compared to the corresponding global-event or slot-based models, thus yielding better computational results, although big-M constraints are used. This model was later extended by Janak et al., ${ }^{35,36}$ allowing tasks to spread over multiple events to accurately account for the utilization of different resources and storage policies. For the comparative study, in this paper, we use a slightly modified version of Ierapetritou and Floudas, ${ }^{29}$ as presented in Appendix A.

### 3.2. Global Event-Based Model of Castro and co-workers. ${ }^{21,22}$ (CBM, CBMN). Castro et

 al. ${ }^{21}$ (CBM) proposed a formulation using RTN representation for short-term scheduling of batch plants. The time horizon is divided into several global events that are common across all units. Binary variables are defined for assigning both start and end times of different tasks to the corresponding global events. Because of the unified treatment of various resources in the RTN framework, no special sequencing constraints are required. All the balances are written in terms of a single excess resource constraint, which implicitly includes the balances on the status and batch amounts of each unit. This model has no big-M constraints except for those that relate the extents of each task to the corresponding binary variables. Because of the provision for end times of tasks to be before the end times of the corresponding time slots, the processing time of each task on a given unit is not exactly represented but has an additional waiting period. Although the authors claimed superiority over the STN based event-driven formulation of Ierapetritou and Floudas, ${ }^{29}$ it was established later (Ierapetritou and Floudas ${ }^{31}$ ) that the claims were based on incorrect data obtained from rounding off the parameter values used. Later, Castro et al. ${ }^{22}$ (CBMN) proposed an improved model by eliminating some of the redundant binary and continuous variables and proposed new timing constraints that result in compact problem statistics and improved relaxed solutions. They compared the results for two different models (MN and MO) with the new and old timing constraints, respectively. On the basis of the request of a reviewer to compare with the new model of Castro et al., ${ }^{22}$ we choose the MN model for comparison because it has fewer constraints and better LP relaxed solution over the MO model. We also compare the performance of the MN model with that of Castro et al. ${ }^{21}$ The models we implemented are reported in Appendix B. Itshould be noted that, in the model of Castro et al., ${ }^{22}$ there is an additional parameter ( $\Delta t$ ) that defines a limit on the maximum number of events over which a task can occur, and it has a significant impact on the solution obtained, the computational time, and the problem statistics. At each event point, we need to iterate over this parameter to get the global optimal solution.
3.3. Unit-Specific Event-Based Model of Giannelos and Georgiadis ${ }^{\mathbf{3 7}}$ (G\&G). The authors proposed an STN represented, unit-specific event-based formulation for short-term scheduling of multipurpose batch plants. This is a slight variation of the model proposed by Ierapetritou and Floudas, ${ }^{29}$ wherein the authors relaxed the task durations using buffer times and implicitly eliminated the various big-M constraints of Ierapetritou and Floudas. ${ }^{29}$ However, the authors introduced special duration and sequencing constraints that effectively transform the nonuniform time grid to a uniform one (global events) for the purposes of material balance and storage constraints. The start times (end times) of the tasks producing/consuming the same state were, respectively, forced to be the same, leading to suboptimal solutions, as observed by Sundaramoorthy and Karimi ${ }^{10}$ and also as demonstrated later in this paper. The model we implemented is reported in Appendix C.
3.4. Global Event-Based Model of Maravelias and Grossmann ${ }^{28}$ (M\&G). This is a recent global event-based model using STN process representation. The model accounts for resource constraints other than equipment (utilities), various storage policies (unlimited, finite, zero wait, and no intermediate storage), and sequence-dependent changeover times and allows for batch mixing/splitting. This model reduces to the case of no resources, and it was used as such for comparison to other approaches (see Maravelias and Grossmann ${ }^{28}$ ). Global event points are used that are common across all units, and tasks are allowed to be processed over multiple events. Different binary variables are used to denote if a task starts, or continues over multiple events, or if it finishes processing a batch at a given event point. Also, a new class of tightening inequalities is proposed for tightening the relaxed LP solutions. The model we implemented for the computational studies in Section 5 is based on the reduction to no resources (refer to Appendix D), and it is included in this comparative study on the grounds that Maravelias and Grossmann ${ }^{28}$ compared it to other continuous-time models without resources. Janak et al. ${ }^{35,36}$ extended the basic event-based formulation of Ierapetritou and Floudas ${ }^{29}$ to allow tasks to extend over multiple events in order to accurately account for different resource constraints and storage policies and provided a comparison for the case of resource constraints. At the request of a reviewer, we employ the
models of Maravelias and Grossmann, ${ }^{28}$ along with the models of Castro et al. ${ }^{22}$ and Janak et al. ${ }^{35,36}$ in a comparative study with resource constraints described in Section 6.
3.5. Slot-Based Model of Sundaramoorthy and Karimi ${ }^{10}$ (S\&K). Among the various slotbased formulations proposed in the literature, this is a recent model available for the short-term scheduling of multipurpose batch plants. The authors claim superior performance for the models they compared with, including those based on global events and that of Giannelos and Georgiadis. ${ }^{37}$ They use generalized recipe diagrams for process representation, wherein a storage task is used to model the mixing and splitting of the same material streams. No resources other than materials and equipment are considered, and transfer and setup times are lumped into the batch processing times of tasks. The time horizon is divided into multiple time slots of varying lengths, and tasks are allowed to continue processing over multiple time slots. For each unit, binary variables are used to assign the beginning of each task to various time slots, and [0,1] continuous variables are used to denote tasks that continue over multiple slots and to denote tasks that release their batch amount at the end of a slot. An additional zero task is defined for modeling idling of units and to occupy extra redundant slots. Even though this model is categorized as slot-based, tasks are allowed to finish before the end of the time slot, making the model inherently similar to the global event-based models, except for the differences in accounting the various balances. Several balances are proposed based on status of each unit, material and storage constraints, and a new way of writing the balance on the time remaining on each unit, leading to a compact model. Some of the examples reported in their paper are not solved to zero integrality gap. In contrast to the authors' claim of 'absolutely' no big-M constraints, the readers can easily verify that there are typographical mistakes in the balances for the batch amount in a unit (constraints 11 and 12 of the original paper; see also Appendix E) which, if corrected, are similar to big-M constraints. Except for these constraints, the resulting model has no other big-M constraints. The model we implemented is reported in Appendix E.

## 4. Description of the Benchmark Examples

In this section, examples without resource constraints such as utility requirements are considered, and additional examples that include resource constraints are discussed later in Section 6. The following three benchmark examples, which have been studied by many authors, are considered
from the short-term scheduling literature ${ }^{10}$ for multipurpose batch plants with variable batch processing times. For simplicity, the process representations and the data for all three examples are shown using the STN representation. The processing time of task $i$ on unit $j$ is assumed to be a linear function, $\alpha_{i j}+\beta_{i j} B$, of its batch size, $B$.
4.1. Example 1. This is a simple motivating example from Sundaramoorthy and Karimi ${ }^{10}$ involving a multipurpose batch plant that requires one raw material and produces two intermediates and one final product. The raw material is processed in three sequential tasks, where the first task is suitable in two units ( J 1 and J 2 ), the second task is suitable in one unit (J3), and the third task is suitable in two units (J4 and J5). The STN for this motivating example is shown in Figure 2.


Figure 2. State-task network representation for example 1.
A task which can be performed in different units is considered as multiple, separate tasks, thus leading to five separate tasks ( $i=1, \ldots, 5$ ), each suitable in one unit. The relevant data ${ }^{10}$ of the constant ( $\alpha_{i j}$ ) and linear ( $\beta_{i j}$ ) coefficients for processing times of different tasks ( $i$ ), the suitable units $(j)$, and their minimum ( $B_{i j}^{\min }$ ) and maximum ( $B_{i j}^{\max }$ ) batch sizes for all three examples considered are shown in Table 1. The storage capacities, initial stock levels, and prices of each state for all three examples are given in Table 2. The initial stock level for all intermediates is assumed to be zero and unlimited storage capacity is assumed for all states.
4. 2. Example 2. This is a standard example for short-term scheduling of multipurpose batch plants and has been studied comprehensively by several authors. Two different products are produced through five processing stages: heating, reactions 1,2 , and 3 , and separation, as shown in the STN representation of the plant flow sheet in Figure 3. Since each of the reaction tasks can take place in two different reactors, each reaction is represented by two separate tasks. The relevant data ${ }^{10,28}$ is shown in Tables 1 and 2. The initial stock level for all intermediates is assumed to be zero and unlimited storage capacity is assumed for all states.

Table 1. Data of Coefficients of Processing Times of Tasks, Limits on Batch Sizes of Units for Examples 1-3

| $\operatorname{Task}(i)$ | $\operatorname{Unit}(j)$ | $\alpha_{i j}$ | $\beta_{i j}$ | $B_{i j}^{\min }(\mathrm{mu})$ | $B_{i j}^{\max }(\mathrm{mu})$ |
| :---: | :---: | :---: | :---: | :---: | :---: |


|  |  | Example 1 |  |  |  |
| ---: | ---: | ---: | ---: | ---: | ---: |
| Task1 $(i=1)$ | Unit1 | 1.333 | 0.01333 | --- | 100 |
| $(i=2)$ | Unit2 | 1.333 | 0.01333 | -- | 150 |
| Task2 $(i=3)$ | Unit3 | 1.000 | 0.00500 | --- | 200 |
| Task3 $(i=4)$ | Unit4 | 0.667 | 0.00445 | -- | 150 |
| $(i=5)$ | Unit5 | 0.667 | 0.00445 | --- | 150 |

Example 2

| Heating $\quad(i=1)$ Heater | 0.667 | 0.00667 | --- | 100 |
| ---: | :--- | :---: | :--- | ---: |
| Reaction1 $(i=2)$ Reactor1 | 1.334 | 0.02664 | --- | 50 |
| $(i=3)$ Reactor2 | 1.334 | 0.01665 | --- | 80 |
| Reaction2 $(i=4)$ Reactor1 | 1.334 | 0.02664 | --- | 50 |
| $(i=5)$ Reactor2 | 1.334 | 0.01665 | --- | 80 |
| Reaction3 $(i=6)$ Reactor1 | 0.667 | 0.01332 | --- | 50 |
| $(i=7)$ Reactor2 | 0.667 | 0.008325 | --- | 80 |
| Separation $(i=8)$ Separator | 1.3342 | 0.00666 | --- | 200 |
|  |  | Example 3 |  |  |
|  |  | 0.00667 | --- | 100 |
| Heating1 $(i=1)$ Heater | 0.667 | 0.01000 | --- | 100 |
| Heating2 $(i=2)$ Heater | 1.000 | 0.01333 | --- | 100 |
| Reaction1 $(i=3)$ Reactor1 | 1.333 | 0.00889 | --- | 150 |
| $(i=4)$ Reactor2 | 1.333 | 0.00667 | --- | 100 |
| Reaction2 $(i=5)$ Reactor1 | 0.667 | 0.00445 | --- | 150 |
| $(i=6)$ Reactor2 | 0.667 | 0.01330 | --- | 100 |
| Reaction3 $(i=7)$ Reactor1 | 1.333 | 0.00889 | --- | 150 |
| $(i=8)$ Reactor2 | 1.333 | 0.00667 | --- | 300 |
| Separation $(i=9)$ Separator | 2.000 | 0.00667 | 20 | 200 |
| Mixing $(i=10)$ Mixer1 | 1.333 | 0.00667 | 20 | 200 |
| $(i=11)$ Mixer2 | 1.333 |  |  |  |

4.3. Example 3. This is a relatively complex example from Sundaramoorthy and Karimi ${ }^{10}$ involving 11 tasks that can be performed in 6 units producing 13 states. The STN for this example is shown in Figure 4. This problem has several common characteristics of a multipurpose batch plant (i.e., a unit can perform either a single task or multiple tasks, a task can be performed in multiple units, etc.). Additionally, some of the intermediates have nonzero initial stock levels and unlimited storage capacity is assumed for all states. The relevant data ${ }^{10}$ is shown in Tables 1 and 2.

Table 2. Data of Storage Capacities, Initial Stock Levels, and Prices of Various States for Examples 1-3 ${ }^{\text {a }}$

| state | example 1 |  |  | example 2 |  |  | example 3 |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | storage capacity (mu) | initial <br> stock <br> (mu) | price <br> (\$/mu) | storage <br> capacity <br> (mu) | initial <br> stock <br> (mu) | price <br> (\$/mu) | storage capacity (mu) | initial <br> stock <br> (mu) | price <br> (\$/mu) |
| S1 | UL | AA | 0 | UL | AA | 0 | UL | AA | 0 |
| S2 | UL | 0 | 0 | UL | AA | 0 | UL | AA | 0 |
| S3 | UL | 0 | 0 | UL | AA | 0 | UL | 0 | 0 |
| S4 | UL | 0 | 5 | UL | 0 | 0 | UL | 0 | 0 |
| S5 |  |  |  | UL | 0 | 0 | UL | 0 | 0 |
| S6 |  |  |  | UL | 0 | 0 | UL | 50 | 0 |
| S7 |  |  |  | UL | 0 | 0 | UL | 50 | 0 |
| S8 |  |  |  | UL | 0 | 10 | UL | AA | 0 |
| S9 |  |  |  | UL | 0 | 10 | UL | 0 | 0 |
| S10 |  |  |  |  |  |  | UL | 0 | 0 |
| S11 |  |  |  |  |  |  | UL | AA | 0 |
| S12 |  |  |  |  |  |  | UL | 0 | 5 |
| S13 |  |  |  |  |  |  | UL | 0 | 5 |

${ }^{a} \mathrm{UL}=$ Unlimited; AA = available as and when required.


Figure 3. State-task network representation for example 2.


Figure 4. State-task network representation for example 3.

## 5. Computational Studies without Resource Constraints

Each of the six short-term scheduling models that are compared for examples without resource constraints are implemented and solved for all the above three examples with respect to two diverse objective functions: maximization of profit and minimization of makespan. The results using maximization of profit are discussed first in Section 5.1, followed by the results for minimization of makespan in Section 5.2. Under each category, several instances of demand distributions and different time horizons are considered for each example as done by Sundaramoorthy and Karimi. ${ }^{10}$ All the resulting MILP models are solved in GAMS distribution 21.1 using CPLEX 8.1.0 on the same computer ( 3 GHz Pentium 4 with 2 GB RAM). The best performing model in each of the instances of different examples is shown on bold face in all the subsequent tables. It should be noted that, in the results by Sundaramoorthy and Karimi ${ }^{10}$ the number of events reported in all the examples is misleading in the comparison tables. They need an additional event $(k=0)$ at the beginning of the time horizon as their numbering of events is from $k=0$ to $K$, although they do not allow any tasks to start at $k=K$. Hence, what they appear to have reported is the number of slots, which is always one less than the total number of global events. In all the subsequent results reported in this study for the model of Sundaramoorthy and Karimi, ${ }^{10}$ we show $n$ event points to represent $n$ - 1 slots for a valid comparison with the other global-event and unit-specific event-based models.
5.1. Maximization of Profit. The computational results for each of the three examples are discussed below for the case of maximization of profit.
5.1.1. Example 1. This motivating example is solved for three different time horizons. The model statistics and computational results for all three cases are shown in Table 3.

Table 3. Model Statistics and Computational Results for Example 1 under Maximization of Profit


In the first scenario, for $H=8 \mathrm{~h}$ (example 1a), both the slot-based and global event-based models require 5 events, while the unit-specific event-based models require only 4 events. All the models
perform equally well with respect to the computational time for this simple case. The model of Castro et al. ${ }^{22}$ (CBMN), solved for $\Delta t=1$, has the best model statistics among the slot-based/global event-based models, while the modified model of Ierapetritou and Floudas ${ }^{29}$ presented in this paper performs the best with respect to the model statistics among all models. In all the results, the models are solved with additional event points until there is no further improvement in the objective function in order to ensure the optimal objective is obtained.

In the second scenario, we consider $H=12 \mathrm{~h}$ (example 1b). In this case, both the slotbased and global event-based models require 9 events, where only 6 events are required by the unit-specific event-based models. However, the model of Giannelos and Georgiadis ${ }^{37}$ gives a suboptimal solution (\$3301.6). This occurs not only for this example but also for several other instances of the other examples considered later, as is also shown recently by Sundaramoorthy and Karimi. ${ }^{10}$ Note that we increased the number of events considered from 6 to 10, and their model is not able to find the global optimal solution (\$3463.6), which is obtained by all the other models. When we remove the special sequencing constraints posed by Giannelos and Georgiadis, ${ }^{37}$ then their model is similar to that of Ierapetritou and Floudas ${ }^{29}$ and gives the global optimal solution. This indicates that the special sequencing constraints for enforcing the same start and finish times for all tasks consuming/producing the same state that were used by Giannelos and Georgiadis ${ }^{37}$ are incorrect and lead to suboptimal solutions. The model of Castro et al. ${ }^{22}(\Delta t=2)$ performs better among the slot-based/global event-based models with respect to the computational time and problem statistics. However, it should be noted that their model ${ }^{22}$ gives a suboptimal solution for $\Delta t$ $=1$, and hence, for a fair comparison with other models, we should add the CPU times and the number of nodes for all instances of $\Delta t$ that need to be tested at each event point. The model of Castro et al. ${ }^{21}$ (CBM) has the largest number of binary variables among all the models. The model of Ierapetritou and Floudas ${ }^{29}$ performs the best among all the models, not only with respect to the model statistics but also with respect to the computational time. This indicates that, although there are big-M constraints in this model, the requirement of fewer events enables this model to outperform all other models.

Similar conclusions hold true for the third scenario of this example, which considers $H=16$ h (example 1c), as is seen in Table 3. For this case, the slot-based/global event-based models require 12 event points compared to the model of Ierapetritou and Floudas, ${ }^{29}$ which requires only 9 events and, hence, is computationally superior to all of the other models. The model of Giannelos and Georgiadis ${ }^{37}$ gives a suboptimal solution (\$4840.9), while all the other models are able to find
the global optimal solution (\$5038.1). The model of Castro et al. ${ }^{22}$ (CBMN) gives a suboptimal solution (\$5000) for $\Delta t=2$, and hence, for fair comparison, we consider the total CPU time of 4997.22 s for $\Delta t=2$ and $\Delta t=3$ at 12 events. So, the model of Castro et al. ${ }^{22}$ performs better among slot-based/global event-based models with respect to the computational time. Among all the models, the model of Maravelias and Grossmann ${ }^{28}$ has the largest number of constraints and nonzeros while the model of Sundaramoorthy and Karimi ${ }^{10}$ has the largest number of continuous variables. The Gantt charts for this case are shown in Figures 5 and 6 for the models of Ierapetritou and Floudas ${ }^{29}$ and Castro et al., ${ }^{22}$ respectively.


Figure 5. Gantt chart for example 1c (9 events) using I\&F model under maximization of profit.


Figure 6. Gantt chart for example 1c (12 events) using CBMN model under maximization of profit.

Note that, for the model of Castro et al. ${ }^{22}$ in Figure 6, there is an additional event at the end at which no task occurs (so a total of 12 events). When we consider an additional slot/event point, the slot-based/global event-based models take excessive CPU times (shown in Table 3), while the unitspecific event-based model of Ierapetritou and Floudas ${ }^{29}$ takes only 21 s to find the same global optimal solution.
5.1.2. Example 2. This example problem is also solved for two different time horizons. The model statistics and computational results for both the cases are shown in Table 4.

Table 4. Model Statistics and Computational Results for Example 2 under Maximization of Profit

| model | event | $\begin{aligned} & \text { ts } \end{aligned} \begin{gathered} \text { CPU } \\ \text { time (s) } \end{gathered}$ | nodes | RMILP <br> (\$) | MILP <br> (\$) | binary variables | continuous variables | constraints | nonzeros |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Example 2a $(H=8)$ |  |  |  |  |  |  |  |  |  |
| S\&K | 5 | 0.07 | 4 | 1730.9 | 1498.6 | 48 | 235 | 249 | 859 |
| M\&G | 5 | 0.16 | 26 | 1730.9 | 1498.6 | 64 | 360 | 826 | 2457 |
| CBM | 5 | 0.07 | 8 | 1812.1 | 1498.6 | 112 | 184 | 322 | 1105 |
| $\operatorname{CBMN}(\Delta \mathrm{t}=1)$ | ) 5 | 0.01 | 4 | 1730.9 | 1498.6 | 32 | 104 | 114 | 439 |
| G\&G | 4 | 0.03 | 14 | 1812.1 | 1498.6 | 32 | 142 | 234 | 820 |
| I\&F | 4 | 0.03 | 13 | 1812.1 | 1498.6 | 18 | 90 | 165 | 485 |
|  | 5 | 0.28 | 883 | 2305.3 | 1498.6 | 26 | 115 | 216 | 672 |
| Example 2b $(H=12)$ |  |  |  |  |  |  |  |  |  |
| S\&K | 7 | 1.93 | 1234 | 3002.5 | 2610.1 | 72 | 367 | 387 | 1363 |
|  | 8 | 29.63 | 16678 | 3167.8 | 2610.3 | 84 | 433 | 456 | 1615 |
|  | 9 | 561.58 | 288574 | 3265.2 | 2646.8 | 96 | 499 | 525 | 1867 |
|  | 10 | 10889.61 | 3438353 | 3315.8 | 2646.8 | 108 | 565 | 594 | 2119 |
|  | 11 | $>67000^{\text {b }}$ | 17270000 | 3343.4 | $2646.8{ }^{\text {a }}$ | 120 | 631 | 663 | 2371 |
| M\&G | 7 | 2.15 | 814 | 3002.5 | 2610.1 | 96 | 526 | 1210 | 4019 |
|  | 8 | 58.31 | 17679 | 3167.8 | 2610.3 | 112 | 609 | 1402 | 4884 |
|  | 9 | 2317.38 | 611206 | 3265.2 | 2646.8 | 128 | 692 | 1594 | 5805 |
|  | 10 | $>67000^{\text {c }}$ | 10737753 | 3315.8 | 2646.8 | 144 | 775 | 1786 | 6782 |
|  | 11 | $>67000^{d}$ | 9060850 | 3343.4 | 2658.5 | 160 | 858 | 1978 | 7815 |
| CBM | 7 | 1.38 | 1421 | 3190.5 | 2610.1 | 216 | 316 | 572 | 2146 |
|  | 8 | 35.81 | 30202 | 3788.3 | 2610.3 | 280 | 394 | 721 | 2791 |
|  | 9 | 1090.53 | 680222 | 4297.9 | 2646.8 | 352 | 480 | 886 | 3519 |
|  | 10 | 40355.97 | 19225950 | 4770.8 | 2646.8 | 432 | 574 | 1067 | 4330 |
|  | 11 | >67000 ${ }^{\text {e }}$ | 13393455 | 5228.7 | $2627.9^{a}$ | 520 | 676 | 1264 | 5224 |
| $\operatorname{CBMN}(\Delta \mathrm{t}=2)$ |  | 0.63 | 1039 | 3045.0 | 2610.1 | 88 | 188 | 224 | 1050 |
|  | 8 | 14.39 | 32463 | 3391.0 | 2610.3 | 104 | 218 | 261 | 1238 |
|  | 9 | 331.72 | 593182 | 3730.5 | 2646.8 | 120 | 248 | 298 | 1426 |
|  | 10 | 4366.09 | 6018234 | 4070.0 | 2646.8 | 136 | 278 | 335 | 1614 |
|  | 11 | $>67000^{f}$ | 80602289 | 4409.5 | $2646.8^{a}$ | 152 | 308 | 372 | 1802 |
| G\&G | 6(to | 11) 0.33 | 701 | 3190.5 | $2564.6{ }^{\text {a }}$ | 48 | 208 | 348 | 1238 |
| I\&F | 7 | 6.19 | 14962 | 3788.3 | 2658.5 | 42 | 165 | 318 | 1046 |
|  | 8 | 105.64 | 211617 | 4297.9 | 2658.5 | 50 | 190 | 369 | 1233 |

${ }^{a}$ Suboptimal solution. ${ }^{b}$ Relative Gap $=1.59 \% .{ }^{c}$ Relative Gap $=3.16 \% .{ }^{d}$ Relative Gap $=5.12 \% .{ }^{e}$ Relative Gap $=$ $28.16 \% .{ }^{f}$ Relative Gap $=2.58 \%$.

In the first scenario, for $H=8 \mathrm{~h}$ (example 2a), both the slot-based and global event-based models require 5 events, while the unit-specific event-based models require only 4 events. All the models perform equally well with respect to the computational time for this simple case. The model of Castro et al. ${ }^{22}$ (CBMN) for $\Delta t=1$ has better problem statistics among slot-based/global event-based models, while the model of Ierapetritou and Floudas ${ }^{29}$ performs the best among all models with
respect to the model statistics. The model of Castro et al. ${ }^{21}$ (CBM) requires the largest number of binary variables, while the model of Maravelias and Grossmann ${ }^{28}$ requires the largest number of continuous variables, constraints, and nonzeros for this case.

In the second scenario, we consider $H=12 \mathrm{~h}$ (example 2 b ). In the paper by Sundaramoorthy and Karimi, ${ }^{10}$ they report the results for this case for the first feasible solution of 7 events only using finite intermediate storage for the intermediate states. In this work, as already mentioned, we solve the problem to its global optimal solution and for zero integrality gap, assuming unlimited intermediate storage for all states. For this case, the slot-based/global eventbased models require at least 11 event points compared to the model of Ierapetritou and Floudas, ${ }^{29}$ which requires only 7 events. The slot-based/global event-based models are not solved until zero integrality gap as they take excessive computational time and because the model of Ierapetritou and Floudas ${ }^{29}$ solves to the global optimal solution in just 6.19 s . The model of Giannelos and Georgiadis ${ }^{37}$ gives a suboptimal solution (\$2564.6). The slot-based/global event-based models take excessive computational time, and only the model of Maravelias and Grossmann ${ }^{28}$ is able to solve to the global optimal solution. The model of Castro et al. ${ }^{21}$ (CBM) has poor LP relaxation and requires more binary variables. The Gantt charts for this case are shown in Figures 7 and 8 for the models of Ierapetritou and Floudas ${ }^{29}$ and Maravelias and Grossmann, ${ }^{28}$ respectively.


Figure 7. Gantt chart for example 2 b (7 events) using I\&F model under maximization of profit.


Figure 8. Gantt chart for example 2 b (11 events) using M\&G model under maximization of profit.

Interestingly, in the Gantt chart of Figure 8 for the model of Maravelias and Grossmann, ${ }^{28}$ it can be observed that, it corresponds to the requirement of a very tiny slot of duration 0.087 h (in the second slot) for the slot-based/global event-based models to find the reported global optimal solution. This is evidenced by the excessive CPU time taken by the slot-based model of Sundaramoorthy and Karimi ${ }^{10}$ for which the global optimal solution is not obtained. However, in the Gantt chart of Figure 7 for the model of Ierapetritou and Floudas, ${ }^{29}$ it is evident that such a slot would not be necessary as they use a unit-specific event-based model. Hence, this case emphasizes the important difference between the slot-based/global event-based models and the unit-specific event-based models. Because of the different alignment of the start times of different units, sometimes the slot-based/global event-based models may require very small slots which can result in a very large number of event points, and may prohibit the realization of global optimal solution in reasonable CPU time compared to the unit-specific event-based models. The unit-specific eventbased models consider the time horizon in a "true" continuous-time form without requiring such tiny time slots and lead to the requirement of a relatively lower number of event points. Thus, this example clearly demonstrates the distinct advantages of the unit-specific event-based models over the slot-based/global event-based models, despite the presence of big-M constraints in the former. The model of Ierapetritou and Floudas ${ }^{29}$ takes only 6.19 s compared to the model of Maravelias and Grossmann, ${ }^{28}$ which takes $>67000$ s for obtaining the same global optimal solution. The model of Sundaramoorthy and Karimi, ${ }^{10}$ although has no big-M constraints, is not able to find the global optimal solution in reasonable CPU time.
5.1.3. Example 3. This relatively complex example is solved for two different time horizons. The model statistics and computational results for both the cases are shown in Table 5. In the first scenario, for $H=8 \mathrm{~h}$ (example 3a), both the slot-based and global event-based models require 7 events, while the unit-specific event-based models require only 5 events. The model of Giannelos and Georgiadis ${ }^{37}$ gives a suboptimal solution (\$1274.5), while all the other models are able to find the global optimal solution (\$1583.4). The model of Castro et al. ${ }^{22}$ (CBMN) for $\Delta t=2$ performs best with respect to the computational time among the slot-based/global event-based models, although it requires more binary variables compared to the model of Sundaramoorthy and Karimi. ${ }^{10}$ The model of Maravelias and Grossmann ${ }^{28}$ has the largest number of continuous variables, constraints, and nonzeros for this case. The model of Ierapetritou and Floudas ${ }^{29}$ performs the best with respect to both the model statistics and the computational time when compared to all of the other models.

Table 5. Model Statistics and Computational Results for Example 3 under Maximization of Profit

| model e | events | $\begin{array}{ll} \text { ts } & \begin{array}{l} \text { CPU } \\ \text { time (s) } \end{array} \end{array}$ | ${ }^{\text {n }}$ nodes | RMILP <br> (\$) | MILP <br> (\$) | binary variables | continuous variables | constraints | nonzeros |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Example 3a ( $H=8$ ) |  |  |  |  |  |  |  |  |  |
| S\&K | 7 | 184.46 | 145888 | 2513.8 | 1583.4 | 102 | 597 | 584 | 2061 |
| M\&G | 7 | 1012.68 | 429949 | 2560.6 | 1583.4 | 132 | 717 | 1667 | 5601 |
| CBM | 7 | 19.82 | 13130 | 2809.4 | 1583.4 | 297 | 433 | 841 | 3049 |
| $\operatorname{CBMN}(\Delta \mathrm{t}=2)$ |  | 6.90 | 10361 | 2606.5 | 1583.4 | 121 | 264 | 343 | 1495 |
| G\&G | 5 | 0.35 | 807 | 2100.0 | $1274.5{ }^{\text {a }}$ | 55 | 244 | 392 | 1335 |
| I\&F | 5 | 0.38 | 1176 | 2100.0 | 1583.4 | 30 | 155 | 303 | 875 |
|  | 6 | 25.92 | 57346 | 2847.8 | 1583.4 | 41 | 190 | 377 | 1139 |
| Example 3b ( $H=12$ ) |  |  |  |  |  |  |  |  |  |
| S\&K | 9 | 372.92 | 94640 | 3867.3 | 3041.3 | 136 | 783 | 792 | 2789 |
|  | 10 | >71000 ${ }^{\text {b }}$ | 12781125 | 4029.7 | 3041.3 | 153 | 876 | 896 | 3153 |
| M\&G | $9$ | 19708.33 | 2254227 | 3867.3 | 3041.3 | 176 | 943 | 2195 | 8114 |
|  | 10 | >71000 ${ }^{\text {c }}$ | 5857914 | 4029.7 | $2981.7^{\text {a }}$ | 198 | 1056 | 2459 | 9492 |
| CBM | 9 | 290.84 | 80123 | 4059.4 | 3041.3 | 484 | 658 | 1307 | 5001 |
|  | 101 | 16416.31 | 3194816 | 4615.6 | 3041.3 | 594 | 787 | 1576 | 6154 |
| $\operatorname{CBMN}(\Delta \mathrm{t}=2)$ |  | 107.97 | 47798 | 3864.3 | 3041.3 | 165 | 348 | 457 | 2031 |
|  | 10 | 1173.82 | 751686 | 4189.8 | 3041.3 | 187 | 390 | 514 | 2299 |
| G\&G | 6 | 1.18 | 2750 | 2871.9 | $2443.2^{a}$ | 66 | 290 | 469 | 1608 |
| I\&F | 7 | 18.33 | 15871 | 3465.6 | 3041.3 | 52 | 225 | 451 | 1403 |
|  | 8 | 50.48 | 41925 | 4059.4 | 3041.3 | 63 | 260 | 525 | 1667 |

Similar conclusions can be drawn for the second scenario where $H=12 \mathrm{~h}$ (example 3 b ). In this case, both the slot-based and global event-based models require 9 events, while only 7 events are required by the unit-specific event-based models. The model of Giannelos and Georgiadis ${ }^{37}$ again gives a suboptimal solution (\$2443.2), while all the other models are able to find the global optimal solution (\$3041.3). The model of Castro et al. ${ }^{22}$ (CBMN) for $\Delta t=2$ performs best for this case with respect to the computational time among the slot-based/global event-based models, although it requires more binary variables compared to the model of Sundaramoorthy and Karimi ${ }^{10}$. The model of Maravelias and Grossmann ${ }^{28}$ has the largest number of continuous variables, constraints, and nonzeros for this case as well. The model of Ierapetritou and Floudas ${ }^{29}$ again performs the best both with respect to the model statistics and the computational time when compared to all the other models. The Gantt charts for this case are shown in Figures 9 and 10 for the models of Ierapetritou and Floudas ${ }^{29}$ and Castro et al., ${ }^{22}$ respectively. When we consider an additional slot/event point, the models of Sundaramoorthy and Karimi ${ }^{10}$ and Maravelias and Grossmann ${ }^{28}$ take excessive CPU times ( $>71000$ s, as shown in Table 5), while the models of Castro and co-workers. ${ }^{21,22}$ perform
better. The model of Ierapetritou and Floudas ${ }^{29}$ again performs the best at higher event points as well.


Figure 9. Gantt chart for example 3b (7 events) using I\&F model under maximization of profit.


Figure 10. Gantt chart for example $3 b$ ( 9 events) using CBMN model under maximization of profit.

The CPU times for representative examples of all the models (except Giannelos and Georgiadis, ${ }^{37}$ as it gives suboptimal solutions) for the objective of maximization of profit are depicted in Figure 11. It should be noted that, the models of Sundaramoorthy and Karimi ${ }^{10}$ and Castro and coworkers. ${ }^{21,22}$ yield suboptimal solutions for example 2 b . The number of binary variables for each model is shown in Figure 12. Thus, with respect to the objective of maximization of profit, in all the instances of the three examples considered, it can be seen that the unit-specific event-based
model of Ierapetritou and Floudas ${ }^{29}$ performs the best in terms of both problem size and computational performance and is orders of magnitude better than the other models. If we consider the cumulative CPU time of increasing events until the same optimal solution is found for each model, then it is evident from Tables 3-5 that, the solution statistics for both the slot-based and global event-based models would be even more inferior compared to the unit-specific event-based model.


Note: S\&K, CBM, and CBMN yield suboptimal solutions for Ex2b

Figure 11. CPU times of different models for maximization of profit.


Figure 12. Number of binary variables in different models for maximization of profit.
5.2. Minimization of Makespan. Finding optimal solutions for problems where the minimization of the makespan is the objective function is reported in the literature to be the most difficult scheduling problem to solve, even for simple examples. Although Sundaramoorthy and

Karimi ${ }^{10}$ claim that their model performs very well for this objective function, it can be seen later that, for some instances, their model also does not find the global optimal solutions (even at higher event points) which are obtained by the unit-specific event-based model of Ierapetritou and Floudas. ${ }^{29}$ In the results reported in Sundaramoorthy and Karimi, ${ }^{10}$ for most of the examples using makespan minimization, each problem is not solved to zero integrality gap, using finite storage for the intermediate states. However, in this work, we solved all the models for all the examples to zero integrality gap assuming unlimited intermediate storage for all states, and by considering an increasing number of event points in order to find the global optimal solutions.

The computational results for each of the three examples are discussed below for the objective of minimization of makespan. The data for all three examples is the same except we consider fixed demands and the time horizon $(H)$ is varied. For all the models that have big-M constraints (Maravelias and Grossmann ${ }^{28}$ and Ierapetritou and Floudas ${ }^{29}$ ), we need to specify the horizon time as well. For fair comparison, we consider the same values of $H$ used by Sundaramoorthy and Karimi. ${ }^{10}$ Note that there is no need to specify $H$ for the model of Giannelos and Georgiadis ${ }^{37}$ when solving makespan minimization problems.
5.2.1. Example 1. This motivating example is solved for two different demand scenarios. The model statistics and computational results for both cases are shown in Table 6. In the first scenario (example 1a), we consider a demand for state $\mathrm{S} 4\left(D_{4}=2000 \mathrm{mu}\right)$, and $H=50 \mathrm{~h}$ is used for the models involving big-M constraints. It can be observed that the optimal solution obtained by the model of Ierapetritou and Floudas ${ }^{29}$ for 12 events $(28.439 \mathrm{~h})$ is better than the best solutions obtained by all other models, even at higher event points. For the models of Sundaramoorthy and Karimi ${ }^{10}$, Maravelias and Grossmann, ${ }^{28}$ and Castro et al., ${ }^{21}$ using 16 events, it takes relatively longer time compared to Castro et al., ${ }^{22}$ even though better solutions are not obtained. The model of Giannelos and Georgiadis ${ }^{37}$ results in a suboptimal solution using $12-15$ event points. For 17 events, the models of Sundaramoorthy and Karimi ${ }^{10}$ and Castro et al. ${ }^{22}$ (CBMN using $\Delta t=2$ ) the optimal solution found is 28.773 h , for which both the models take more than 80000 s . The model of Ierapetritou and Floudas ${ }^{29}$ outperforms all the other models in terms of computational time and problem size and finds the global optimal solution of 27.881 h using 14 events with a CPU time of just 41.89 s. The Gantt chart for this case is shown in Figure 13 for the model of Ierapetritou and Floudas. ${ }^{29}$

Table 6. Model Statistics and Computational Results for Example 1 under Minimization of Makespan

| model events | H | $\begin{aligned} & \text { CPU } \\ & \text { time (s) } \end{aligned}$ | nodes | RMILP <br> (h) | MILP <br> (h) | binary variables | continuous variables | constraints | nonzeros |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Example 1a ( $\left.D_{4}=2000 \mathrm{mu}\right)$ |  |  |  |  |  |  |  |  |  |
| S\&K 13 | -- | 1.18 | 362 | 27.126 | 29.772 | 120 | 615 | 624 | 2074 |
| 14 | -- | 31.54 | 15622 | 25.702 | 29.772 | 130 | 665 | 678 | 2253 |
| 15 | -- | 728.05 | 400789 | 25.142 | 29.439 | 140 | 715 | 732 | 2432 |
| 16 | -- | 37877.69 | 12064418 | 24.871 | 29.106 | 150 | 765 | 786 | 2611 |
| 17 | -- | $>80000^{\text {b }}$ | 17279722 | 24.716 | $28.773{ }^{a}$ | 160 | 815 | 840 | 2790 |
| M\&G 13 | 50 | 2.19 | 394 | 27.126 | 29.772 | 120 | 556 | 1485 | 6056 |
| 14 |  | 645.06 | 139488 | 25.335 | 29.772 | 130 | 601 | 1605 | 6786 |
| 15 |  | 25253.81 | 5273904 | 25.024 | 29.439 | 140 | 646 | 1725 | 7551 |
| 16 |  | $>90000^{\text {c }}$ | 11258561 | 24.834 | $29.106{ }^{\text {a }}$ | 150 | 691 | 1845 | 8351 |
| CBM 13 | -- | 0.50 | 6 | 23.313 | 29.772 | 450 | 568 | 1066 | 4404 |
| 14 | -- | 14.90 | 4262 | 21.049 | 29.772 | 520 | 647 | 1219 | 5095 |
| 15 | -- | 2163.55 | 454549 | 19.049 | 29.439 | 595 | 731 | 1382 | 5836 |
| 16 | -- | 64850.69 | 9852772 | 17.049 | $29.106{ }^{\text {a }}$ | 675 | 820 | 1555 | 6627 |
| $\operatorname{CBMN}(\Delta \mathrm{t}=1) 13$ | -- | 0.02 | 0 | 27.126 | 29.772 | 60 | 191 | 239 | 824 |
| $(\Delta t=1) 14$ | -- | 0.11 | 65 | 25.824 | 29.772 | 65 | 206 | 258 | 892 |
| $(\Delta t=1) 15$ | -- | 0.28 | 417 | 25.358 | 29.772 | 70 | 221 | 277 | 960 |
| ( $\Delta \mathrm{t}=2) 15$ | -- | 235.90 | 236250 | 19.049 | 29.439 | 135 | 286 | 407 | 1605 |
| $(\Delta t=2) 16$ | -- | 27994.64 | 23426601 | 17.049 | 29.106 | 145 | 306 | 436 | 1723 |
| $(\Delta t=2) 17$ | -- | $>80000{ }^{\text {d }}$ | 80105289 | 15.049 | $28.773{ }^{a}$ | 155 | 326 | 465 | 1841 |
| G\&G 12 | -- | 0.03 | 0 | 27.126 | 29.772 | 60 | 228 | 367 | 1108 |
| 15 | -- | 1.87 | 3529 | 25.064 | $29.772^{a}$ | 75 | 285 | 457 | 1387 |
| $\mathbf{I \& F}$ | 50 | 0.12 | 208 | 24.236 | 28.439 | 50 | 160 | 253 | 732 |
| 13 |  | 2.26 | 7863 | 24.236 | 27.903 | 55 | 174 | 276 | 801 |
| 14 |  | 41.89 | 134961 | 24.236 | 27.881 | 60 | 188 | 299 | 870 |
| 15 |  | 950.64 | 2693556 | 24.236 | 27.881 | 65 | 202 | 322 | 939 |
| Example 1b $\left(D_{4}=4000 \mathrm{mu}\right)$ |  |  |  |  |  |  |  |  |  |
| S\&K 23 | -- | 101.03 | 34598 | 51.362 | 56.432 | 220 | 1115 | 1164 | 3864 |
| 24 | -- | 15814.03 | 4164921 | 49.939 | $56.432{ }^{\text {a }}$ | 230 | 1165 | 1218 | 4043 |
| M\&G 23 | 100 | 21974.42 | 2525960 | 51.362 | 56.432 | 220 | 1006 | 2685 | 14931 |
| 24 |  | $>90000^{\circ}$ | 5129168 | 49.572 | $57.765^{a}$ | 230 | 1051 | 2805 | 16011 |
| CBM 23 | -- | 6.09 | 185 | 43.313 | 56.432 | 1375 | 1583 | 3046 | 13564 |
| 24 | -- | 2016.50 | 136348 | 41.049 | $56.432{ }^{a}$ | 1495 | 1712 | 3299 | 14755 |
| $\operatorname{CBMN}(\Delta \mathrm{t}=1) 23$ | -- | 0.05 | 0 | 51.362 | 56.432 | 110 | 341 | 429 | 1504 |
| $(\Delta t=2) 24$ | -- | 0.20 | 72 | 50.061 | 56.432 | 115 | 356 | 448 | 1572 |
| $(\Delta t=2) 25$ | -- | $>80000{ }^{f}$ | 34358380 | 39.049 | $56.099^{a}$ | 235 | 486 | 697 | 2785 |
| $\text { G\&G } \quad 22$ | -- | 0.07 | 0 | 51.362 | 56.432 | 110 | 418 | 667 | 2038 |
| 24 | -- | 1.53 | 1707 | 49.594 | $56.432{ }^{\text {a }}$ | 120 | 456 | 727 | 2224 |
| I\&F 22 | 100 | 6.48 | 19019 | 48.473 | 52.433 | 100 | 300 | 483 | 1422 |
| 23 |  | 384.12 | 832372 | 48.473 | 52.072 | 105 | 314 | 506 | 1491 |

${ }^{a}$ Suboptimal solution. ${ }^{b}$ Relative Gap $=4.22 \% .{ }^{c}$ Relative Gap $=7.38 \%$. ${ }^{d}$ Relative Gap $=0.12 \% .{ }^{e}$ Relative Gap $=$ $11.01 \% .{ }^{f}$ Relative Gap $=2.18 \%$.

Similar conclusions hold true for the second scenario (example 1b) where the demand is $D_{4}=4000$ mu , and $H=100 \mathrm{~h}$ is used for the models involving big-M constraints. The model of Ierapetritou
and Floudas ${ }^{29}$ outperforms the other models and finds the global optimal solution of 52.072 h using 23 events with a CPU time of 384.12 s.


Figure 13. Gantt chart for example 1a (14 events) using I\&F model under minimization of makespan.
5.2.2. Example 2. This problem is solved with demands for states S8 and S9 ( $D_{8}=D_{9}=200$ mu ) and $H=50 \mathrm{~h}$ is used for the models involving big-M constraints. The model statistics and computational results are shown in Table 7.

Table 7. Model Statistics and Computational Results for Example 2 under Minimization of Makespan

| model | events | H | $\begin{aligned} & \text { CPU } \\ & \text { time (s) } \end{aligned}$ | nodes | RMILP <br> (h) | MILP <br> (h) | binary variables | continuous variable | onstraints | nonzeros |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Example $2\left(D_{8}=D_{9}=200 \mathrm{mu}\right)$ |  |  |  |  |  |  |  |  |  |  |
| S\&K | 9 | -- | 10.98 | 5378 | 18.685 | 19.789 | 96 | 556 | 528 | 1936 |
|  | 10 | -- | 519.35 | 142108 | 18.685 | 19.340 | 108 | 622 | 597 | 2188 |
|  | 11 | -- | 11853.03 | 2840768 | 18.685 | 19.340 | 120 | 688 | 666 | 2440 |
| M\&G | 9 | 50 | 66.55 | 15674 | 18.685 | 19.789 | 128 | 693 | 1598 | 5869 |
|  | 10 |  | 5693.53 | 1066939 | 18.685 | 19.340 | 144 | 776 | 1790 | 6850 |
|  | 11 |  | $>80000{ }^{\text {b }}$ | 5019315 | 18.685 | 19.340 | 160 | 859 | 1982 | 7887 |
| CBM | 9 | -- | 7.75 | 6426 | 12.555 | 19.789 | 352 | 481 | 888 | 3584 |
|  | 10 | -- | 727.23 | 441130 | 9.889 | 19.340 | 432 | 575 | 1069 | 4403 |
|  | 11 | -- | 32258.74 | 13776145 | 7.223 | 19.340 | 520 | 677 | 1266 | 5305 |
| $\operatorname{CBMN}(\Delta \mathrm{t}=1) 9$ |  | -- | 0.71 | 1809 | 18.685 | 19.789 | 64 | 193 | 216 | 872 |
| $(\Delta t=1) 10$ |  | -- | 50.49 | 134189 | 18.685 | 19.789 | 72 | 215 | 241 | 979 |
|  | $(\Delta t=2) 10$ | -- | 56.11 | 109917 | 15.654 | 19.340 | 136 | 279 | 337 | 1623 |
| G\&G | ( $\Delta \mathrm{t}=2$ )11 | -- | 5535.27 | 8389012 | 12.988 | 19.340 | 152 | 309 | 374 | 1811 |
|  | 8 | -- | 1.97 | 3804 | 12.555 | 19.789 | 64 | 274 | 475 | 1675 |
|  | 10 | -- | 1614.35 | 1182082 | 10.475 | $19.789^{a}$ | a 80 | 340 | 589 | 2093 |
| I\&F | 8 | 50 | 0.78 | 1008 | 12.738 | 19.764 | 45 | 190 | 367 | 1211 |
|  | 9 |  | 74.26 | 111907 | 12.477 | 19.340 | 53 | 215 | 418 | 1398 |
|  | 10 |  | 1672.11 | 2079454 | 12.435 | 19.340 | 61 | 240 | 469 | 1585 |

For this case, all the models except one are able to find the optimal solution of 19.34 h ; however, the model of Ierpateritou \& Floudas ${ }^{29}$ requires 1 less event point. The model of Giannelos and Georgiadis ${ }^{37}$ did not find the optimal solution using 8-10 event points. The model of Maravelias and Grossmann ${ }^{28}$ has the largest computational time and the largest number of continuous variables, constraints, and nonzeros. The model of Castro et al. ${ }^{22}$ (CBMN) performs better among slot-based/global event-based models as it takes an overall of 106.6 s using 10 events (for $\Delta t=1$ and $\Delta t=2$ ). The model of Ierapetritou and Floudas ${ }^{29}$ has the least number of binary and continuous variables and performs the best with respect to the computational time as well using only 9 events. The Gantt charts for this case are shown in Figures 14 and 15 for the models of Ierapetritou and Floudas ${ }^{29}$ and Castro et al., ${ }^{22}$ respectively.


Figure 14. Gantt chart for example 2 ( 9 events) using I\&F model under minimization of makespan.


Figure 15. Gantt chart for example 2 ( 10 events) using CBMN model under minimization of makespan.
5.2.3. Example 3. This relatively complex example is solved for two different demand scenarios. The model statistics and computational results for both the cases are shown in Table 8. In the first scenario (example 3a), we consider demands for state S12 and S13 ( $D_{12}=100 \mathrm{mu}, D_{13}=$ 200 mu ), and $H=50 \mathrm{~h}$ is used for the models involving big-M constraints. All the models are solved for an increasing number of event points. The slot-based/global event-based models require 11 events to find the optimal solution of 13.367 h . The model of Maravelias and Grossmann ${ }^{28}$ takes excessive CPU time (>80 000 s with $3.1 \%$ gap) and has the largest number of continuous variables,
constraints, and nonzeros. The model of Castro et al. ${ }^{21}$ solves faster among the slot-based/global event-based models using 11 events, although it has very poor LP relaxation. There is no improvement in the model of Giannelos and Georgiadis ${ }^{37}$ from 7-9 events, and each yields a suboptimal solution. The model of Ierapetritou \& Floudas ${ }^{29}$ requires just 7 events and outperforms the other models in terms of both exceptional computational performance ( 0.38 s vs 2514.97 s taken by Castro et al. ${ }^{21}$ ) and least problem size. The Gantt charts for this case are shown in Figures 16 and 17 for the models of Ierapetritou and Floudas ${ }^{29}$ and Castro et al., ${ }^{21}$ respectively.

Table 8. Model Statistics and Computational Results for Example 3 under Minimization of Makespan

| model | events | H | CPU <br> time (s) | nodes | RMILP <br> (h) | MILP <br> (h) | binary <br> variables variables | continuous costraints nonzeros |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |


| Example 3a ( $D_{12}=100 \mathrm{mu}, D_{13}=200 \mathrm{mu}$ ) |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| S\&K | 8 | -- | 0.28 | 36 | 12.317 | 14.366 | 119 | 690 | 689 | 2425 |
|  | 9 | -- | 13.32 | 5156 | 11.621 | 13.589 | 136 | 783 | 793 | 2789 |
|  | 10 | -- | 226.83 | 53789 | 11.417 | 13.532 | 153 | 876 | 897 | 3153 |
|  | 11 | -- | 4340.65 | 821194 | 11.335 | 13.367 | 170 | 969 | 1001 | 3517 |
|  | 12 | -- | >80000 ${ }^{1}$ | 11858901 | 11.295 | 13.367 | 187 | 1062 | 1105 | 3881 |
| M\&G | 8 | 50 | 1.15 | 316 | 12.317 | 14.366 | 154 | 831 | 1937 | 6905 |
|  | 9 |  | 126.77 | 21366 | 11.621 | 13.589 | 176 | 944 | 2201 | 8208 |
|  | 10 |  | 3949.36 | 605450 | 11.417 | 13.532 | 198 | 1057 | 2465 | 9592 |
|  | 11 |  | >80000 ${ }^{2}$ | 7481387 | 11.335 | 13.367 | 220 | 1170 | 2729 | 11057 |
| CBM | 8 | -- | 0.62 | 68 | 10.941 | 14.366 | 385 | 541 | 1064 | 4044 |
|  | 9 | -- | 5.89 | 2762 | 8.941 | 13.589 | 484 | 659 | 1309 | 5090 |
|  | 10 | -- | 53.42 | 22452 | 6.941 | 13.532 | 594 | 788 | 1578 | 6254 |
|  | 11 | -- | 2514.97 | 673460 | 4.941 | 13.367 | 715 | 928 | 1871 | 7536 |
|  | 12 | -- | $>80000^{3}$ | 20380858 | 3.825 | 13.367 | 847 | 1079 | 2188 | 8936 |
| $\operatorname{CBMN}(\Delta \mathrm{t}=2)$ | 8 | -- | 0.23 | 67 | 12.192 | 14.366 | 143 | 307 | 402 | 1776 |
| $(\Delta t=2) 9$ |  | -- | 2.23 | 2566 | 10.192 | 13.589 | 165 | 349 | 459 | 2044 |
| $(\Delta t=2) 10$ |  | -- | 14.73 | 17426 | 8.192 | 13.532 | 187 | 391 | 516 | 2312 |
| $(\Delta t=2) 11$ |  | -- | 312.07 | 326752 | 6.192 | 13.532 | 209 | 433 | 573 | 2580 |
| $(\Delta t=3) 11$ |  | -- | 20230.89 | 16842943 | 6.192 | 13.367 | 297 | 521 | 725 | 3494 |
| $(\Delta t=3) 12$ |  | -- | 11547.29 | 5054232 | 4.635 | 13.367 | 330 | 574 | 801 | 3877 |
| G\&G | 7 | -- | 0.25 | 338 | 11.066 | 14.616 | 77 | 336 | 558 | 1902 |
|  | 9 | -- | 3.36 | 3960 | 10.167 | $14.616^{a}$ | 99 | 428 | 712 | 2448 |
| I\&F | 7 | 50 | $0.38$ | 458 | 11.066 | 13.367 | 52 | 225 | 452 | 1413 |
|  | 8 |  | 2.89 | 3506 | 10.000 | $13.367$ | 63 | 260 | 526 | 1677 |
| Example 3b ( $\left.D_{12}=D_{13}=250 \mathrm{mu}\right)$ |  |  |  |  |  |  |  |  |  |  |
| S\&K | 11 | -- | 981.01 | 226238 | 14.535 | $17.357^{a}$ | 170 | 969 | 1001 | 3517 |
| M\&G | 11 | 100 | 62724.36 | 5802875 | 14.535 | $17.357^{a}$ | 220 | 1170 | 2729 | 11057 |
| CBM | 11 | -- | 38.14 | 9627 | 10.722 | $17.357{ }^{\text {a }}$ | 715 | 928 | 1871 | 7536 |
| $\operatorname{CBMN}(\Delta \mathrm{t}=2)$ |  | -- | 31.57 | 28079 | 12.494 | $17.357{ }^{\text {a }}$ | 209 | 433 | 573 | 2580 |
| G\&G | 10 | -- | 59.26 | 84970 | 12.763 | $18.978{ }^{\text {a }}$ | 110 | 474 | 789 | 2721 |
| I\&F | 10 | 100 | 2.50 | 2668 | 12.500 | 17.025 | 85 | 330 | 674 | 2205 |
|  | 11 |  | 396.58 | 424617 | 12.500 | 17.025 | 96 | 365 | 748 | 2469 |

${ }^{\text {a }}$ Suboptimal solution; Relative Gap: 1.01 \% ${ }^{1}$, 3.055 \% $^{2}$, $3.29 \%^{3}$

When we consider an additional slot/event point, except the model of Castro et al., ${ }^{22}$ the slotbased/global event-based models take excessive CPU times (>80 000 s , as shown in Table 8) while the unit-specific event-based model of Ierapetritou and Floudas ${ }^{29}$ takes only 2.89 s to find the same global optimal solution.


Figure 16. Gantt chart for example 3a (7 events) using I\&F model under minimization of makespan.


Figure 17. Gantt chart for example 3a (11 events) using CBM model under minimization of makespan.

Similar conclusions hold true for the second scenario (example 3b), where the demands are $D_{12}=$ $D_{13}=250 \mathrm{mu}$ and $H=100 \mathrm{~h}$ is used for the models involving big-M constraints. All the slotbased/global event-based models require 11 events to find the suboptimal solution of 17.357 h . The model of Giannelos and Georgiadis ${ }^{37}$ gives a suboptimal solution (18.978 h) using 10 events.

The model of Castro et al. ${ }^{22}$ using 11 events (for $\Delta t=2$ ) solves faster among the slot-based/global event-based models, but it provides a suboptimal solution. However, the model of Ierapetritou \& Floudas ${ }^{29}$ finds the global optimal solution of 17.025 h in 2.5 s and, hence, outperforms the other models.

The CPU times for representative examples of all the models (except Giannelos and Georgiadis ${ }^{37}$ as it gives suboptimal solutions) for the objective of minimization of makespan are depicted in Figure 18. The number of binary variables for each model is shown in Figure 19.


Note: S\&K, M\&G, CBM, and CBMN yield suboptimal solutions for Ex1a
Figure 18. CPU times of different models for minimization of makespan.


Note: S\&K, M\&G, CBM, and CBMN yield suboptimal solutions for Ex1a
Figure 19. Number of binary variables in different models for minimization of makespan.

It should be noted that, all the slot-based/global event-based models of Sundaramoorthy and Karimi ${ }^{10}$, Maravelias and Grossmann, ${ }^{28}$ and Castro and co-workers ${ }^{21,22}$ yield suboptimal solutions for example 1a, example 1 b , and example 3 b . It can be observed that, for the objective of minimization of makespan as well, the unit-specific event-based model of Ierapetritou \& Floudas ${ }^{29}$ outperforms all the other models by orders of magnitude and is able to find global optimal solutions in all cases. If we consider the cumulative CPU time of increasing events until the global optimal solution is found for each model, then it is evident from Tables 6-8 that the solution statistics for both the slot-based and global event-based models would be even more inferior compared to the unit-specific event-based model.

## 6. Computational Studies with Resource Constraints

Even though a comparative study of approaches with resource constraints was provided in Janak et al., ${ }^{35,36}$ at the request of a reviewer, we consider here additional examples that include resource constraints such as utility requirements and mixed storage policies. For the global event-based formulations, the models of Maravelias and Grossmann ${ }^{28}$ and Castro et al., ${ }^{22}$ and for the unitspecific event-based formulations, the model of Janak et al., ${ }^{35,36}$ are considered in the comparative study.
6.1. Example 4. This example, which includes resource constraints, variable batch sizes and processing times, and utility requirements, was solved by Maravelias and Grossmann ${ }^{28}$ and Janak et al. ${ }^{35}$ The STN for this example is shown in Figure 20, and the corresponding data ${ }^{28,35}$ is given in Tables 9 and 10.


Figure 20. STN for example 4

Table 9. State Related Data for Example 4

|  | F1 | F2 | I1 | I2 | I3 | P1 | P2 |
| :--- | ---: | ---: | ---: | ---: | :--- | :--- | :--- |
| $S T_{s}^{\text {max }}(\mathrm{kg})$ | 1000 | 1000 | 200 | 100 | 500 | 1000 | 1000 |
| $S T_{s}^{0}(\mathrm{~kg})$ | 400 | 400 | 0 | 0 | 0 | 0 | 0 |
| $\operatorname{price}_{s}(\$ / \mathrm{kg})$ | 0 | 0 | 0 | 0 | 0 | 30 | 40 |

Table 10. Task Related Data for Example $4^{a}$

|  |  | T1 |  | T2 |  | T3 |  | T4 |  |  | T1 |  | T2 |  | T3 |  | T4 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| cap ${ }^{\text {min }}$ | cap ${ }^{\text {max }}$ | $\alpha$ | $\beta$ | $\alpha$ | $\beta$ | $\alpha$ | $\beta$ | $\alpha$ |  | $\beta$ | $\gamma_{i H S}$ | $\delta_{i H S}$ | $\gamma_{i C W}$ | $\delta_{i C l}$ | $\gamma_{i H S} \delta^{\prime}$ | $\delta_{i H S}$ | $\gamma_{i C W} \delta_{i C W}$ |
| R1 40 | 80 | 0.5 | 0.025 | 0.75 | 0.03 |  |  |  |  |  | 6 | 0.25 | 4 | 0.3 |  |  |  |
| R2 25 | 50 | 0.5 | 0.4 | 0.75 | 0.06 |  |  |  |  |  | 4 | 0.25 | 3 | 0.3 |  |  |  |
| R3 40 | 80 |  |  |  |  | 0.25 | 0.01 | 0.5 | 50. | 0.025 |  |  |  |  | 8 | 0.4 | 40.5 |

${ }^{a}$ cap $^{\text {min }} /$ cap $^{\text {max }}$ in kg, $\alpha$ in h, $\beta$ in $\mathrm{h} / \mathrm{kg}, \gamma$ in $\mathrm{kg} / \mathrm{min}$, and $\delta$ in $\mathrm{kg} /$ min per kg of batch.

There are two types of reactors available for the process (types I and II), with two reactors of type I (R1 and R2) and one reactor of type II (R3) with four reactions suitable in them. Reactions T1 and T2 require a type I reactor, whereas reactions T3 and T4 require a type II reactor. Additionally, reactions T1 and T3 are endothermic, where the required heat is provided by steam (HS) available in limited amounts. Reactions T2 and T4 are exothermic, and the required cooling water (CW) is also available in limited amounts. Each reactor allows variable batch sizes, where the minimum batch size is half the capacity of the reactor. The processing times and the utility requirements include a fixed time and a variable term that is proportional to the batch size. The processing times are set so that the minimum batch size is processed in $60 \%$ of the time needed for the maximum batch size. For the raw materials and final products, unlimited storage is available, while for the intermediates, finite storage is available. Two different cases of this example studied in the literature ${ }^{28,35}$ are considered that differ in the resource availability. In the first case (example 4a), we assume that the availability of both HS and CW is $40 \mathrm{~kg} / \mathrm{min}$, and in the second case (example 4b), it is $30 \mathrm{~kg} / \mathrm{min}$. Also, two different objective functions, maximization of profit and minimization of makespan, are considered.
6.1.1. Maximization of Profit. For the objective of maximization of profit and a time horizon of 8 h , the optimal solution is $\$ 5904.0$ in the first case (example 4 a ) and $\$ 5227.778$ in the second case (example 4b). The computational results in terms of the model statistics and the CPU times are reported in Table 11 for the models of Maravelias and Grossmann ${ }^{28}$ (M\&G), Janak et al. ${ }^{35}$ (JLF), and Castro et al. ${ }^{22}$ (CBMN).
6.1.2. Minimization of Makespan. For the objective of minimization of makespan, the optimal solution is 8.5 h in the first case (example 4 a ) and 9.025 h in the second case (example 4 b ). The computational results in terms of the model statistics and the CPU times are reported in Table 12 for the models of Maravelias and Grossmann ${ }^{28}$ (M\&G), Janak et al. ${ }^{35}$ (JLF), and Castro et al. ${ }^{22}$ (CBMN). For the models involving big-M constraints, ${ }^{28,35}$ a common value of $M=10$ is used.

Table 11. Model Statistics and Computational Results for Example 4 under Maximization of Profit

| model events | $\begin{aligned} & \text { CPU } \\ & \text { time (s) } \end{aligned}$ | nodes | RMILP <br> (\$) | MILP <br> (\$) | binary <br> variables | continuous variables | constraints | nonzeros |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Example 4a |  |  |  |  |  |  |  |  |
| M\&G 7 | 1.22 | 680 | 8870.5 | 5904.0 | 72 | 545 | 1082 | 4184 |
| $\operatorname{CBMN}(\Delta \mathrm{t}=1) 7$ | 0.30 | 376 | 8875.4 | $5482.04{ }^{\text {a }}$ | 36 | 140 | 175 | 741 |
| $(\Delta t=2) 7$ | 1.07 | 1312 | 10396.7 | 5904.0 | 66 | 170 | 250 | 1216 |
| JLF 6 | 1.03 | 294 | 10981.8 | 5904.0 | 45 | 273 | 1304 | 4606 |
| Example 4b |  |  |  |  |  |  |  |  |
| M\&G 6 | 0.27 | 67 | 7267.1 | 5227.8 | 60 | 470 | 925 | 3411 |
| $\operatorname{CBMN}(\Delta \mathrm{t}=1) 6$ | 0.09 | 96 | 7685.7 | $5000.0^{a}$ | 30 | 121 | 148 | 622 |
| $(\Delta t=2) 6$ | 0.16 | 112 | 8360.3 | 5227.8 | 54 | 145 | 208 | 1002 |
| JLF 5 | 0.15 | 26 | 6414.7 | 5227.8 | 33 | 220 | 1028 | 3265 |
| ${ }^{a}$ Suboptimal solution |  |  |  |  |  |  |  |  |

Table 12. Model Statistics and Computational Results for Example 4 under Minimization of Makespan


For both the objective functions, the unit-specific event-based model of Janak et al. ${ }^{35}$ requires 1 event point less and has the least number of binary variables compared to the global event-based models of Maravelias and Grossmann ${ }^{28}$ and Castro et al. ${ }^{22}$. The model of Castro et al. ${ }^{22}$ (using $\Delta t=$ 2) requires the least number of continuous variables, constraints and nonzeros. It should be noted
that the model of Castro et al. ${ }^{22}$ (CBMN) yields suboptimal solution for $\Delta t=1$ in both the cases and hence, the overall CPU time and the number of nodes (for both $\Delta t=1$ and $\Delta t=2$ ) should be considered.
6. 2. Example 5. This example comprises of resource constraints, mixed storage policies, variable batch sizes and processing times, and utility requirements that was solved by Maravelias and Grossmann, ${ }^{28}$ Janak et al., ${ }^{35}$ and Castro et al. ${ }^{22}$. The STN for this example is shown in Figure 21, and the relevant data is given in Tables 13 and 14.


Figure 21. STN for example 5

Table 13. State Related Data for Example 5


Table 14. Task Related Data for Example $5^{a}$

|  | T1 | T2 | T3 | T4 | T5 | T6 | T7 | T8 | T9 | T10 |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :--- |
| unit | U 1 | U 2 | U 3 | U 1 | U 4 | U 4 | U | U6 | U5 | U 6 |
| cap $^{\max }$ | 5 | 8 | 6 | 5 | 8 | 8 | 3 | 4 | 3 | 4 |
| $\alpha$ | 2 | 1 | 1 | 2 | 2 | 2 | 4 | 2 | 2 | 3 |
| utility | LPS | CW | LPS | HPS | LPS | HPS | CW | LPS | CW | CW |
| $\gamma$ | 3 | 4 | 4 | 3 | 8 | 4 | 5 | 5 | 5 | 3 |
| $\delta$ | 2 | 2 | 3 | 2 | 4 | 3 | 4 | 3 | 3 | 3 |
| ${ }^{a}$ Cap $^{\max }$ in $\mathrm{kg}, ~$ | $\alpha$ in h, $\gamma$ in $\mathrm{kg} / \mathrm{min}$, and $\delta$ in $\mathrm{kg} /$ min per kg of batch. |  |  |  |  |  |  |  |  |  |

The plant consists of 6 units involving 10 processing tasks and 14 states. Unlimited intermediate storage (UIS) is available for raw materials F1 and F2, intermediates I1 and I2, and final products P1-P3 and WS. Finite intermediate storage (FIS) is available for states S3 and S4, while no
intermediate storage (NIS) is available for states S2 and S6, and a zero-wait (ZW) policy applies for states S1 and S5. There are three different renewable utilities: cooling water (CW), lowpressure steam (LPS), and high-pressure steam (HPS). Tasks T2, T7, T9, and T10 require CW; tasks T1, T3, T5, and T8 require LPS; and tasks T 4 and T 6 require HPS. The maximum availabilities of CW, LPS, and HPS are 25, 40, and $20 \mathrm{~kg} / \mathrm{min}$, respectively. The objective function is maximization of profit, and two instances of time horizons of 12 h (example 5 a ) and 14 h (example 5b) are considered.

For the objective of maximization of profit and a time horizon of 12 h , the optimal solution is $\$ 13000$ in the first case (example 5a), and for a time horizon of 14 h , the optimal solution is $\$ 16350$ in the second case (example 5b). The computational results in terms of the model statistics and the CPU times are reported in Table 15 for the models of Maravelias and Grossmann ${ }^{28}$ (M\&G), Janak et al. ${ }^{35}$ (JLF), and Castro et al. ${ }^{22}$ (CBMN).

Table 15. Model Statistics and Computational Results for Example 5 under Maximization of Profit

| model events | $\begin{aligned} & \text { CPU } \\ & \text { time (s) } \end{aligned}$ | nodes | RMILP <br> (\$) | MILP <br> (\$) | binary variables | continuous variables | constraints | nonzeros |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Example 5a $(H=12)$ |  |  |  |  |  |  |  |  |
| M\&G 9 | 63.63 | 18150 | 18423.5 | 13000 | 160 | 993 | 2184 | 7282 |
| $\operatorname{CBMN}(\Delta \mathrm{t}=1) 9$ | 0.26 | 291 | 18388.7 | $10000{ }^{\text {a }}$ | 80 | 320 | 464 | 1618 |
| $(\Delta t=2) 9$ | 4.35 | 3767 | 21063.3 | 13000 | 150 | 390 | 688 | 2668 |
| JLF 8 | 1.33 | 115 | 24000 | 13000 | 109 | 743 | 3100 | 11309 |
| Example 5b $(H=14)$ |  |  |  |  |  |  |  |  |
| M\&G 8 | 0.89 | 94 | 18648.6 | 16350 | 140 | 875 | 1923 | 6163 |
| $\operatorname{CBMN}(\Delta \mathrm{t}=1) 8$ | 0.06 | 1 | 18473.7 | $15000{ }^{\text {a }}$ | 70 | 286 | 409 | 1422 |
| $(\Delta t=2) 8$ | 0.15 | 10 | 18696.4 | 16350 | 130 | 346 | 601 | 2322 |
| JLF 7 | 0.42 | 48 | 18960.4 | 16350 | 91 | 643 | 2690 | 9258 |
| ${ }^{a}$ Suboptimal solution |  |  |  |  |  |  |  |  |

It should be noted that, for the model of Janak et al., ${ }^{35}$ two additional storage tasks are defined explicitly, while for the models of Maravelias and Grossmann ${ }^{28}$ and Castro et al., ${ }^{22}$ no storage tasks are required. The unit-specific event-based model of Janak et al. ${ }^{35}$ requires 1 event point less and has the least number of binary variables compared to the global event-based models of Maravelias and Grossmann ${ }^{28}$ and Castro et al. ${ }^{22}$ The model of Castro et al. ${ }^{22}$ (using $\Delta t=2$ ) requires the least number of continuous variables, constraints, and nonzeros. It should be noted that the model of Castro et al. ${ }^{22}$ (CBMN) yields a suboptimal solution for $\Delta t=1$ in both cases, and hence, the overall CPU time and the number of nodes (for both $\Delta t=1$ and $\Delta t=2$ ) need to be considered.

## 7. Conclusion

In this paper, we compare and assess the performance of various continuous-time models proposed in the literature for short-term scheduling of multipurpose batch plants. These models are broadly classified into three distinct categories: slot-based, global event-based, and unit-specific eventbased formulations. On the basis of our implementation, the models are compared using several benchmark example problems from the literature. Two different objective functions, maximization of profit and minimization of makespan, are considered, and the models are compared with respect to different metrics such as problem size (in terms of the number of variables and constraints), computational times (on the same computer), and number of nodes taken to reach zero integrality gap. It is observed that, both the slot-based and global event-based models always require the same number of event points, while the unit-specific event-based models require less event points to solve a problem to global optimality. Thus, the unit-specific event-based models result in smaller problem sizes compared to both slot-based and global event-based models and are computationally superior. In all the examples considered for the objective of maximization of profit, the model of Castro et al. ${ }^{22}$ performs better among the slot-based/global event-based models, and it usually requires the smaller number of continuous variables and constraints, while the model of Maravelias and Grossmann ${ }^{28}$ generally has the largest number of constraints and nonzeros. For example 2 b , the models of Sundaramoorthy and Karimi, ${ }^{10}$ and Castro and co-workers ${ }^{21,22}$ yield suboptimal solutions. In constrast, for the objective of minimization of makespan, all the slot-based/global event-based models perform weakly in most of the instances of the examples compared to the unitspecific event-based model of Ierapetritou and Floudas. ${ }^{29}$ For examples 1a, 1b, and 3b Sundaramoorthy and Karimi, ${ }^{10}$ Maravelias and Grossmann, ${ }^{28}$ and Castro and co-workers. ${ }^{21,22}$ result in suboptimal solutions. The model of Giannelos and Georgiadis ${ }^{37}$ yields suboptimal solutions most of the time because of the special sequencing constraints enforced in their model. The unit-specific event-based model of Ierapetritou and Floudas ${ }^{29}$ attains the global optimal solution in all examples, and performs the best in terms of both computational performance and problem size. When resource constraints such as utility requirements are considered in the additional two examples it is observed that the unit-specific event-based model of Janak et al. ${ }^{35}$ requires 1 less event point and the minimum number of binary variables compared to the global event-based models of Maravelias and Grossmann ${ }^{28}$ and Castro et al. ${ }^{22}$

## Appendix A: Unit-Specific Event-Based Model of Ierapetritou and Floudas ${ }^{29}$ (I\&F)

The following is the model used in this paper for the unit-specific event-based formulation of Ierapetritou and Floudas. ${ }^{29}$

For the objective of maximization of profit:

$$
\begin{align*}
& \text { Max Profit }=\sum_{s} \operatorname{price}_{s}\left(S T(s, N)+\sum_{i \in \rho_{s i}>0} \rho_{s i} \sum_{j \in s u i t_{j j}} b(i, j, N)\right)  \tag{A.1}\\
& \sum_{i \in s u i_{i j}} w(i, j, n) \leq 1 \quad \forall j, n  \tag{A.2}\\
& w(i, j, n) B_{i j}^{\min } \leq b(i, j, n) \leq w(i, j, n) B_{i j}^{\max } \quad \forall i, j \in \text { suit }_{i j}, \forall n  \tag{A.3}\\
& S T(s, n)=S T(s, n-1)+\sum_{i \in \rho_{s i}>0} \rho_{s i} \sum_{j \in s u u_{j i}} b(i, j, n-1)+\sum_{i \in \rho_{s i}<0} \rho_{s i} \sum_{j \in s s u t_{j}} b(i, j, n) \quad \forall s, n  \tag{A.4}\\
& t s(i, j, n+1) \geq t s\left(i^{\prime}, j, n\right)+\alpha_{i^{\prime} j} w\left(i^{\prime}, j, n\right)+\beta_{i^{\prime} j} b\left(i^{\prime}, j, n\right) \quad \forall i, i^{\prime}, j \in \text { suit }_{i j}, \text { suit }_{i^{\prime} j}, \forall n<N  \tag{A.5}\\
& t s(i, j, n+1) \geq t s\left(i^{\prime}, j^{\prime}, n\right)+\alpha_{i^{\prime} j^{\prime}} w\left(i^{\prime}, j^{\prime}, n\right)+\beta_{i^{\prime} j^{\prime}} b\left(i^{\prime}, j^{\prime}, n\right)-H\left(1-w\left(i^{\prime}, j^{\prime}, n\right)\right) \\
& \forall s, i, i^{\prime}, j, j^{\prime} \in \text { suit }_{i j}, \text { suit }_{i^{\prime} j^{\prime}}, i \neq i^{\prime}, j \neq j^{\prime}, \rho_{s i}<0, \rho_{s i^{\prime}}>0, \forall n<N \text { (A.6) } \\
& t s(i, j, N)+\alpha_{i j} w(i, j, N)+\beta_{i j} b(i, j, N) \leq H \quad \forall i, j \in \text { suit }_{i j}  \tag{A.7}\\
& t s(i, j, n) \leq H \quad \forall i, j \in \operatorname{suit}_{i j}, \forall n  \tag{A.8}\\
& S T(s, n) \leq S T_{s}^{\max } \quad \forall s \in F I S, \forall n  \tag{A.9}\\
& w(i, j, n)=b(i, j, n)=t s(i, j, n)=0 \quad \forall i, j \in \text { suit }_{i j}=0 \tag{A.10}
\end{align*}
$$

For the objective of minimization of makespan:

$$
\begin{align*}
& \operatorname{Min} \quad M S  \tag{A.11}\\
& \sum_{s}\left(S T(s, N)+\sum_{i \in \rho_{s i}>0} \rho_{s i} \sum_{j \in s u u t_{i j}} b(i, j, N)\right) \geq \text { Demand }_{s}  \tag{A.12}\\
& t s(i, j, N)+\alpha_{i j} w(i, j, N)+\beta_{i j} b(i, j, N) \leq M S \quad \forall i, j \in \text { suit }_{i j} \tag{A.13}
\end{align*}
$$

The model for makespan minimization is composed of constraints A.2-A. 6 and A.9-A.13. The original model of Ierapetritou and Floudas ${ }^{29}$ is slightly modified here with some of the dependent variables being eliminated, and the constraints for the same task in the same unit and different tasks in the same unit are combined into one equation in eq. A.5. Also, in contrast to the original model, the only big-M constraints are in constraint A.6. This led to improved LP relaxations in some of the examples. If the problem involves sequence-dependent changeovers, then the constraint A. 5 will also have big-M terms. Additionally, tasks that cannot occur at certain events are identified and the corresponding variables are fixed to zero in our implementation.

## Appendix B: Global Event-Based Models of Castro and co-workers ${ }^{21,22}$ (CBM, CBMN)

The following is the model used in this paper for the global event-based formulation of Castro et al. ${ }^{21}$ (CBM).

For the objective of maximization of profit:
Max Profit $=\sum_{r}$ price $_{r} R(r, t=|T|)$
$T\left(t^{\prime}\right)-T(t) \geq \alpha_{i} \bar{N}\left(i, t, t^{\prime}\right)+\beta_{i} \bar{\xi}\left(i, t, t^{\prime}\right) \quad \forall i, t, t^{\prime} \in t^{\prime}>t$
$N(i, t)=\sum_{t^{\prime}>t} \bar{N}\left(i, t, t^{\prime}\right) \quad \forall i, t \in t<|T|$
$\xi(i, t)=\sum_{t^{\prime}>t} \bar{\xi}\left(i, t, t^{\prime}\right) \quad \forall i, t \in t<|T|$
$V_{i}^{\text {min }} N(i, t) \leq \xi(i, t) \leq V_{i}^{\text {max }} N(i, t) \quad \forall i, t \in t<|T|$
$V_{i}^{\min } \bar{N}\left(i, t, t^{\prime}\right) \leq \bar{\xi}\left(i, t, t^{\prime}\right) \leq V_{i}^{\max } \bar{N}\left(i, t, t^{\prime}\right) \quad \forall i, t, t^{\prime} \in t^{\prime}>t, t<|T|$
$R(r, t)=\left.R_{r}^{0}\right|_{t=1}+\left.R(r, t-1)\right|_{t>1}+\sum_{i}\left(\mu_{r i} N(i, t)+v_{r i} \xi(i, t)\right)+\sum_{i} \sum_{t^{\prime}<t}\left(\overline{\mu_{r i}} \bar{N}\left(i, t t^{\prime}, t\right)+\overline{v_{r i}} \bar{\xi}\left(i, t^{\prime}, t\right)\right) \quad \forall r, t$
$R_{r}^{\min } \leq R(r, t) \leq R_{i}^{\max } \quad \forall r, t$
$T(t) \leq H \quad \forall t$
$T(t)=0 \quad \forall t=1$
$\bar{N}\left(i, t, t^{\prime}\right)=\bar{\xi}\left(i, t, t^{\prime}\right)=0 \quad \forall t^{\prime}=1$ or $t^{\prime} \leq t$
$N(i, t)=\xi(i, t)=\bar{N}\left(i, t, t^{\prime}\right)=\bar{\xi}\left(i, t, t^{\prime}\right)=0 \quad \forall t=|T|$
For the objective of minimization of makespan:
Min $M S$
$R(r, t) \geq$ Demand $_{r} \quad t=|T|$
$T(t) \leq M S \quad t=|T|$
The model for makespan minimization is composed of constraints B.2-B. 8 and B.10-B.15.
The following is the model used in this paper for the global event-based formulation of Castro et al. ${ }^{22}$ (CBMN). The variables $N(i, t)$ and $\xi(i, t)$ are eliminated from the model of Castro et al., ${ }^{21}$ and for each event we have an additional iteration over a parameter $\Delta t$.

For the objective of maximization of profit:
Max Profit $=\sum_{r}$ price $_{r} R(r, t=|T|)$
$T\left(t^{\prime}\right)-T(t) \geq \sum_{i} \overline{\mu_{r i}}\left(\alpha_{i} \bar{N}\left(i, t, t^{\prime}\right)+\beta_{i} \bar{\xi}\left(i, t, t^{\prime}\right)\right) \quad \forall r \in R^{E Q}, t, t^{\prime}, t<t^{\prime} \leq \Delta t+t, t \neq|T|$
$V_{i}^{\min } \bar{N}\left(i, t, t^{\prime}\right) \leq \bar{\xi}\left(i, t, t^{\prime}\right) \leq V_{i}^{\max } \bar{N}\left(i, t, t^{\prime}\right) \quad \forall i, t, t^{\prime}, t<t^{\prime} \leq \Delta t+t, t \neq|T|$

$$
\begin{align*}
& R(r, t)=\left.R_{r}^{0}\right|_{t=1}+\left.R(r, t-1)\right|_{t>1}+\sum_{i} \sum_{t<t^{\prime} \leq \Delta t+t}\left(\mu_{r i} \bar{N}\left(i, t, t^{\prime}\right)+v_{r i} \bar{\xi}\left(i, t, t^{\prime}\right)\right) \\
& \quad+\sum_{i} \sum_{t-\Delta t t^{\prime} t^{\prime} t}\left(\overline{\mu_{r i}} \bar{N}\left(i, t^{\prime}, t\right)+\overline{v_{r i}} \bar{\xi}\left(i, t t^{\prime}, t\right)\right) \quad \forall r, t
\end{aligned} \quad \begin{aligned}
& \begin{array}{l}
R_{r}^{\min } \leq R(r, t) \leq R_{i}^{\max } \quad \forall r, t \\
T(t) \leq H \quad \forall t
\end{array}  \tag{B.19}\\
& \begin{array}{l}
T(t)=0 \quad \forall t=1 \\
\bar{N}\left(i, t, t^{\prime}\right)=\bar{\xi}\left(i, t, t^{\prime}\right)=0 \quad \forall t^{\prime}=1 \text { or } \quad t^{\prime} \leq t \quad \text { or } \quad \forall t=|T|
\end{array} \tag{B.20}
\end{align*}
$$

The model for makespan minimization is composed of constraints B.13-B.15, B.17-B.20, and B.22-B.23.

For zero-wait tasks, the following constraint needs to be added:

$$
\begin{array}{r}
T\left(t^{\prime}\right)-T(t) \leq H\left(1-\sum_{i \in I^{2 W}} \overline{\mu_{r i}} \bar{N}\left(i, t, t^{\prime}\right)\right)+\sum_{i \in I^{2 W}} \overline{\mu_{r i}}\left(\alpha_{i} \bar{N}\left(i, t, t^{\prime}\right)+\beta_{i} \bar{\xi}\left(i, t, t^{\prime}\right)\right)  \tag{B.24}\\
\forall r \in R^{E Q}, t, t^{\prime}, t<t^{\prime} \leq \Delta t+t, t \neq|T|
\end{array}
$$

## Appendix C: Unit-Specific Event-Based Model of Giannelos and Georgiadis ${ }^{37}$ (G\&G)

The following is the model used in this paper for the unit-specific event-based formulation of Giannelos and Georgiadis. ${ }^{37}$

For the objective of maximization of profit:
Max profit $=\sum_{s}$ price $_{s} \operatorname{STF}(s)$

$$
\begin{equation*}
\sum_{i \in s u i t_{j j}} x(i, n) \leq 1 \quad \forall j, n \tag{C.1}
\end{equation*}
$$

$x(i, n) B_{i}^{\min } \leq b(i, n) \leq x(i, n) B_{i}^{\max } \quad \forall i, n$
$S T(s, n)=S T(s, n-1)+\sum_{i \in \rho_{s i}>0} \rho_{s i} b(i, n-1)+\sum_{i \in \rho_{s i}<0} \rho_{s i} b(i, n) \quad \forall s, n$
$\operatorname{STF}(s)=S T(s, N)+\sum_{i \in \rho_{s i}>0} \rho_{s i} b(i, N) \quad \forall s$
$\tau(i, n) \geq \tau(i, n-1)+\theta(i, n)+\alpha_{i} x(i, n)+\beta_{i} b(i, n) \quad \forall i, n$
$\tau(i, n)=\tau\left(i^{\prime}, n\right) \quad \forall s, i, i^{\prime}, n \in i \neq i^{\prime}, \rho_{s i}>0, \rho_{s i^{\prime}}>0, i=\operatorname{HEAD}\left(I_{s}^{p}\right)$
$\tau(i, n)-\theta(i, n)-\left(\alpha_{i} x(i, n)+\beta_{i} b(i, n)\right)=\tau\left(i^{\prime}, n\right)-\theta\left(i^{\prime}, n\right)-\left(\alpha_{i} x(i, n)+\beta_{i} b(i, n)\right)$
$\forall s, i, i^{\prime}, n \in i \neq i^{\prime}, \rho_{s i}<0, \rho_{s i^{\prime}}<0, i=\operatorname{HEAD}\left(I_{s}^{c}\right)$
$\tau(i, n-1)=\tau\left(i^{\prime}, n\right)-\theta\left(i^{\prime}, n\right)-\left(\alpha_{i} x\left(i^{\prime}, n\right)+\beta_{i} b\left(i^{\prime}, n\right) \quad \forall s, i, i^{\prime}, n \in i=\operatorname{HEAD}\left(I_{s}^{p}\right), i^{\prime}=\operatorname{HEAD}\left(I_{s}^{c}\right)\right.$
$\tau(i, n)=\tau\left(i^{\prime}, n\right) \quad \forall j, i, i^{\prime}, n \in i \neq i^{\prime}$, suit $_{i j}$, suit $_{i^{\prime} j}, i=\operatorname{HEAD}(j)$
$\tau(i, N) \leq H \quad \forall i$
$S T(s, n) \leq S T_{s}^{\max } \quad \forall s \in F I S, \forall n$

For the objective of minimization of makespan:

$$
\begin{array}{ll}
\operatorname{Min} M S & \\
S T F(s) \geq \text { Demand }_{s} & \forall s \\
\tau(i, N) \leq M S & \forall i \tag{C.15}
\end{array}
$$

The model for makespan minimization consists of constraints C.2-C. 10 and C.12-C.15.

Appendix D: Global Event-Based Model of Maravelias and Grossmann ${ }^{28}$ (M\&G)
The following is the model used in this paper for the global event-based formulation of Maravelias and Grossmann. ${ }^{28}$

For the objective of maximization of profit:

$$
\begin{align*}
& \text { Max Profit }=\sum_{s} \text { price }_{s} S T(s, N)  \tag{D.1}\\
& \sum_{i \in s s i t_{j}} W s(i, n) \leq 1 \quad \forall j, n  \tag{D.2}\\
& \sum_{i \in s u i_{j i}} W f(i, n) \leq 1 \quad \forall j, n  \tag{D.3}\\
& \sum_{n} W s(i, n)=\sum_{n} W f(i, n) \quad \forall i  \tag{D.4}\\
& \sum_{i \in s s i t_{j j}} \sum_{n \leq n}\left(W s\left(i, n^{\prime}\right)-W f\left(i, n^{\prime}\right)\right) \leq 1 \quad \forall j, n  \tag{D.5}\\
& D(i, n)=\alpha_{i} W s(i, n)+\beta_{i} B s(i, n) \quad \forall i, n  \tag{D.6}\\
& T f(i, n) \leq T s(i, n)+D(i, n)+H(1-W s(i, n)) \quad \forall i, n  \tag{D.7}\\
& T f(i, n) \geq T s(i, n)+D(i, n)-H(1-W s(i, n)) \quad \forall i, n  \tag{D.8}\\
& T f(i, n)-T f(i, n-1) \leq H W s(i, n) \quad \forall i, n>1  \tag{D.9}\\
& T f(i, n)-T f(i, n-1) \geq D(i, n) \quad \forall i, n>1  \tag{D.10}\\
& T s(i, n)=T(n) \quad \forall i, n  \tag{D.11}\\
& T f(i, n-1) \leq T(n)+H(1-W f(i, n)) \quad \forall i, n>1  \tag{D.12}\\
& W_{s}(i, n) B_{i}^{\text {min }} \leq B s(i, n) \leq W s(i, n) B_{i}^{\text {max }} \quad \forall i, n  \tag{D.13}\\
& B_{i}^{\min }\left(\sum_{n^{\prime}<n} W s\left(i, n^{\prime}\right)-\sum_{n^{\prime} \leq n} W f\left(i, n^{\prime}\right)\right) \leq B p(i, n) \leq B_{i}^{\max }\left(\sum_{n^{\prime}<n} W s\left(i, n^{\prime}\right)-\sum_{n^{\prime} \leq n} W f\left(i, n^{\prime}\right)\right) \forall i, n  \tag{D.14}\\
& B s(i, n-1)+B p(i, n-1)=B p(i, n)+B f(i, n) \quad \forall i, n>1  \tag{D.16}\\
& B^{I}(i, s, n)=\rho_{s i} B s(i, n) \quad \forall i, n, \forall s \in S I(i)  \tag{D.17}\\
& B^{I}(i, s, n) \leq B_{i}^{\text {max }} \rho_{s i} W s(i, n) \quad \forall i, n, \forall s \in S I(i)
\end{align*}
$$

$$
\begin{align*}
& B^{o}(i, s, n)=\rho_{s i} B f(i, n) \quad \forall i, n, \forall s \in S O(i)  \tag{D.19}\\
& B^{o}(i, s, n) \leq B_{i}^{\max } \rho_{s i} W f(i, n) \quad \forall i, n, \forall s \in S O(i)  \tag{D.20}\\
& S T(s, n)=S T(s, n-1)+\sum_{i \in O(s)} B^{O}(i, s, n)-\sum_{i \in I(s)} B^{I}(i, s, n) \quad \forall s, n>1  \tag{D.21}\\
& T(n+1) \geq T(n) \quad \forall n<N  \tag{D.22}\\
& \sum_{i \in \text { suit }_{j}} \sum_{n} D(i, n) \leq H \quad \forall j  \tag{D.23}\\
& \sum_{i \in s u i_{i j}} \sum_{n \geq n} D\left(i, n^{\prime}\right) \leq H-T(n) \quad \forall j, n  \tag{D.24}\\
& \sum_{i \in s u i_{i j}} \sum_{n^{\prime} \leq n}\left(\alpha_{i} W f\left(i, n^{\prime}\right)+\beta_{i} B f\left(i, n^{\prime}\right)\right) \leq T(n) \quad \forall j, n  \tag{D.25}\\
& T s(i, n) \leq H \quad \forall i, n  \tag{D.26}\\
& T f(i, n) \leq H \quad \forall i, n  \tag{D.27}\\
& S T(s, n) \leq S T_{s}^{\max } \quad \forall s \in F I S, \forall n  \tag{D.28}\\
& T(n)=W f(i, n)=B f(i, n)=B^{o}(i, s, n)=0 \quad \forall n=1  \tag{D.29}\\
& W s(i, n)=B s(i, n)=D(i, n)=B p(i, n)=B^{I}(i, s, n)=0 \quad \forall n=N  \tag{D.30}\\
& T(N)=H \tag{D.31}
\end{align*}
$$

For the objective of minimization of makespan:
Min $M S$
$S T(s, N) \geq$ Demand $_{s} \quad \forall s$
$T(N)=M S$
$\sum_{i \in s u i_{i j}} \sum_{n} D(i, n) \leq M S \quad \forall j$
$\sum_{i \in s u i_{i j}} \sum_{n \geq n} D\left(i, n^{\prime}\right) \leq M S-T(n) \quad \forall j, n$
The model for makespan minimization uses constraints D.2-D.22, D.25-D.30, and D.32-D.36.
For zero-wait tasks, the following constraints are added:
$T f(i, n-1) \geq T(n)-H(1-W f(i, n)) \quad \forall i \in I^{Z W}, n>1$
When utility requirements are considered, the following constraints are added:

$$
\begin{array}{ll}
R^{I}(i, r, n)=\gamma_{i r} W s(i, n)+\delta_{i r} B s(i, n) & \forall i, r, n \\
R^{o}(i, r, n)=\gamma_{i r} W f(i, n)+\delta_{i r} B f(i, n) & \forall i, r, n \\
R(r, n)=R(r, n-1)-\sum_{i} R^{o}(i, r, n-1)+\sum_{i} R^{I}(i, r, n) \quad \forall r, n \\
R(r, n) \leq R_{r}^{\max } \quad \forall r, n & \tag{D.41}
\end{array}
$$

## Appendix E: Slot-Based Model of Sundaramoorthy and Karimi ${ }^{10}$ (S\&K)

The following is the model used in this paper for the slot-based formulation of Sundaramoorthy and Karimi. ${ }^{10}$ Here, the set of tasks (I) also includes an idle task ' $i 0$ 'that is suitable on all units.

For the objective of maximization of profit:
Max Profit $=\sum_{s}$ price $_{s} S T(s, K)$
$\sum_{k} S L(k) \leq H$
$Z(j, k)=\sum_{i \in \text { suit }_{j}} Y(i, j, k) \quad \forall j, 0 \leq k<K$
$Y(i, j, k) B_{i j}^{\min } \leq B(i, j, k) \leq Y(i, j, k) B_{i j}^{\max } \quad \forall i>0, j \in$ suit $_{i j}, 0 \leq k<K$
$y(i, j, k)=y(i, j, k-1)+Y(i, j, k-1)-Y E(i, j, k) \quad \forall i, j \in \operatorname{suit}_{i j}, 0<k<K$
$Z(j, k)=\sum_{i \in s u s i_{j}} Y E(i, j, k) \quad \forall j, 0<k<K$
$t(j, k+1) \geq t(j, k)+\sum_{i \in s u t_{i j}}\left(\alpha_{i j} Y(i, j, k)+\beta_{i j} B(i, j, k)\right)-S L(k+1) \quad \forall j, k<K$
$b(i, j, k)=b(i, j, k-1)+B(i, j, k-1)-B E(i, j, k) \quad \forall i>0, j \in$ suit $_{i j}, k>0$
$y(i, j, k) B_{i j}^{\min } \leq b(i, j, k) \leq y(i, j, k) B_{i j}^{\max } \quad \forall i>0, j \in \operatorname{suit}_{i j}, 0<k<K$
$Y E(i, j, k) B_{i j}^{\min } \leq B E(i, j, k) \leq Y E(i, j, k) B_{i j}^{\max } \quad \forall i>0, j \in$ suit $_{i j}, 0<k \leq K$
$t(j, k) \leq \sum_{i \in s u i_{j}} \alpha_{i j} y(i, j, k)+\beta_{i j} b(i, j, k) \quad \forall j, 0<k<K$
$S T(s, k)=S T(s, k-1)+\sum_{j} \sum_{i \in s u i t_{j}, i \neq 0, \rho_{s}>0} \rho_{s i} B E(i, j, k)+\sum_{j} \sum_{i \in s u u_{i}, i \neq 0, \rho_{s i}<0} \rho_{s i} B(i, j, k) \quad \forall s, k$
$S T(s, k) \leq S T_{s}^{\max } \quad \forall s \in F I S, \forall k$
$S L(k) \leq \max _{j}\left[\max _{i \in s u t_{i j}}\left(\alpha_{i j}+\beta_{i j} B_{i j}^{\max }\right)\right] \quad \forall k>0$
$t(j, k) \leq \max _{i \in s u t_{i j}}\left(\alpha_{i j}+\beta_{i j} b_{i j}^{\max }\right) \quad \forall j, k$
$Y(i, j, k)=y(i, j, k)=b(i, j, k)=B(i, j, k)=0 \quad \forall i, j \in$ suit $_{i j}=0$ or $k=K$
$Y E(i, j, k)=y(i, j, k)=b(i, j, k)=B E(i, j, k)=0 \quad \forall i, j \in \operatorname{suit}_{i j}=0$ or $k=0$
$Z(j, k)=t(j, k)=0 \quad \forall j, k=K$
$t(j, k)=0 ; S L(k)=0 \quad \forall k=0$
$0 \leq y(i, j, k), Y E(i, j, k), Z(j, k) \leq 1$
For the objective of minimization of makespan:
$\operatorname{Min} M S=\sum_{k=1}^{K} S L(k)$
$S T(s, K) \geq$ Demand $_{s} \quad \forall s$

The model for makespan minimization consists of constraints E.3-E.22. The constraints E. 9 and E. 10 are misprinted in the original paper (constraints 11 and 12 of Sundaramoorthy and Karimi ${ }^{10}$ ), in which they were written as follows:

$$
\begin{align*}
& B_{i j}^{\min } \leq b(i, j, k) \leq B_{i j}^{\max }-y(i, j, k) \quad \forall i>0, j \in \text { suit }_{i j}, 0<k<K  \tag{E.23}\\
& Y E(i, j, k) B_{i j}^{\min } \leq B E(i, j, k) \leq B_{i j}^{\max }-Y E(i, j, k) \quad \forall i>0, j \in \text { suit }_{i j}, 0<k \leq K \tag{E.24}
\end{align*}
$$

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## References

(1) Floudas, C. A.; Lin, X. Continuous-time versus discrete-time approaches for scheduling of chemical processes: A review. Comput. Chem. Eng. 2004, 28, 2109.
(2) Floudas, C. A.; Lin, X. Mixed integer linear programming in process scheduling: Modeling, algorithms, and applications. Ann. Oper. Res. 2005, 139, 131.
(3) Pinto, J. M.; Grossmann, I. E. Optimal cyclic scheduling of multistage continuous multiproduct plants. Comput. Chem. Eng. 1994, 18, 797.
(4) Pinto, J. M.; Grossmann, I. E. A continuous time mixed integer linear programming model for short term scheduling of multistage batch plants. Ind. Eng. Chem. Res. 1995, 34, 3037.
(5) Pinto, J. M.; Grossmann, I. E. An alternate MILP model for short-term scheduling of batch plants with preordering constraints. Ind. Eng. Chem. Res. 1996, 35, 338.
(6) Pinto, J. M.; Grossmann, I. E. A logic-based approach to scheduling problems with resource constraints. Comput. Chem. Eng. 1997, 21, 801.
(7) Karimi, I. A.; McDonald, C. M. Planning and scheduling of parallel semi-continuous processes. 2. Short-term scheduling. Ind. Eng. Chem. Res. 1997, 36, 2701.
(8) Lamba, N.; Karimi, I. A. Scheduling parallel production lines with resource constraints. 1. Model formulation. Ind. Eng. Chem. Res. 2002, 41, 779.
(9) Lamba, N.; Karimi, I. A. Scheduling parallel production lines with resource constraints. 2. Decomposition algorithm. Ind. Eng. Chem. Res. 2002, 41, 790.
(10) Sundaramoorthy, A.; Karimi, I. A. A simpler better slot-based continuous-time formulation for short-term scheduling in multipurpose batch plants. Chem. Eng. Sci. 2005, 60, 2679.
(11) Zhang, X.; Sargent, R. W. H. The optimal operation of mixed production facilities - A general formulation and some approaches for the solution. Comput. Chem. Eng. 1996, 20, 897.
(12) Zhang, X.; Sargent, R. W. H. The optimal operation of mixed production facilities Extensions and improvements. Comput. Chem. Eng. 1998, 22, 1287.
(13) Mockus, L.; Reklaitis, G. V. Mathematical programming formulation for scheduling of batch operations based on nonuniform time discretization. Comput. Chem. Eng. 1997, 21, 1147.
(14) Mockus, L.; Reklaitis, G. V. Continuous time representation approach to batch and continuous process scheduling. 1. MINLP formulation. Ind. Eng. Chem. Res. 1999, 38, 197.
(15) Mockus, L.; Reklaitis, G. V. Continuous time representation approach to batch and continuous process scheduling. 2. Computational issues. Ind. Eng. Chem. Res. 1999, 38, 204.
(16) Schilling, G.; Pantelides, C. C. A simple continuous-time process scheduling formulation and a novel solution algorithm. Comput. Chem. Eng. 1996, 20, S1221.
(17) Schilling, G.; Pantelides, C. C. Optimal periodic scheduling of multipurpose plants. Comput. Chem. Eng. 1999, 23, 635.
(18) Mendez, C. A.; Henning, G. P.; Cerda, J. Optimal scheduling of batch plants satisfying multiple product orders with different due-dates. Comput. Chem. Eng. 2000, 24, 2223.
(19) Mendez, C. A.; Cerda, J. An MILP continuous-time framework for short-term scheduling of multipurpose batch processes under different operation strategies. Optim. Eng. 2003, 4, 7.
(20) Mendez, C. A.; Henning, G. P.; Cerda, J. An MILP continuous-time approach to short-term scheduling of resource-constrained multistage flowshop batch facilities. Comput. Chem. Eng. 2001, 25, 701.
(21) Castro, P.; Barbosa-Povoa, A. P. F. D.; Matos, H. An improved RTN continuous-time formulation for the short-term scheduling of multipurpose batch plants. Ind. Eng. Chem. Res. 2001, 40, 2059.
(22) Castro, P. M.; Barbosa-Povoa, A. P.; Matos, H. A.; Novais, A. Q. Simple continuous-time formulation for short-term scheduling of batch and continuous processes. Ind. Eng. Chem. Res., 2004, 43, 105.
(23) Mendez, C. A.; Cerda, J. Optimal scheduling of a resource-constrained multiproduct batch plant supplying intermediates to nearby end-product facilities. Comput. Chem. Eng. 2000, 24, 369.
(24) Majozi, T.; Zhu, X. X. Novel continuous-time MILP formulation for multipurpose batch plants. 1. Short-term scheduling. Ind. Eng. Chem. Res. 2001, 40, 5935.
(25) Lee, K.; Park, H. I.; Lee, I. A novel nonuniform discrete time formulation for short-term scheduling of batch and continuous processes. Ind. Eng. Chem. Res. 2001, 40, 4902.
(26) Burkard, R. E.; Fortuna, T.; Hurkens, C. A. J. Makespan minimization for chemical batch processes using nonuniform time grids. Comput. Chem. Eng. 2002, 26, 1321.
(27) Wang, S.; Guignard, M. Redefining event variables for efficient modeling of continuoustime batch processing. Ann. Oper. Res. 2002, 116, 113.
(28) Maravelias, C. T.; Grossmann, I. E. New general continuous-time state-task network formulation for short-term scheduling of multipurpose batch plants. Ind. Eng. Chem. Res. 2003, 42, 3056.
(29) Ierapetritou, M. G.; Floudas, C. A. Effective continuous-time formulation for short-term scheduling: 1. Multipurpose batch processes. Ind. Eng. Chem. Res. 1998, 37, 4341.
(30) Ierapetritou, M.G.; Floudas, C.A. Effective continuous-time formulation for short-term scheduling: 2. Continuous and semi-continuous processes. Ind. Eng. Chem. Res. 1998, 37, 4360.
(31) Ierapetritou, M. G.; Floudas, C. A. Comments on "An Improved RTN continuous-time formulation for the short-term scheduling of multipurpose batch plants." Ind. Eng. Chem. Res. 2001, 40, 5040.
(32) Ierapetritou, M. G.; Hene, T. S.; Floudas, C. A. Effective continuous-time formulation for short-term scheduling: 3. Multiple intermediate due dates. Ind. Eng. Chem. Res. 1999, 38, 3446.
(33) Lin, X.; Floudas, C. A. Design, synthesis and scheduling of multipurpose batch plants via an effective continuous-time formulation. Comput. Chem. Eng. 2001, 25, 665.
(34)Lin, X.; Chajakis, E. D.; Floudas, C. A. Scheduling of tanker lightering via a novel continuous-time optimization framework. Ind. Eng. Chem. Res. 2003, 42, 4441.
(35) Janak, S. L.; Lin, X.; Floudas, C. A. Enhanced continuous-time unit-specific event-based formulation for short-term scheduling of multipurpose batch processes: Resource constraints and mixed storage policies. Ind. Eng. Chem. Res. 2004, 42, 2516.
(36) Janak, S. L.; Lin, X.; Floudas, C. A. Comments on "Enhanced continuous-time unitspecific event-based formulation for short-term scheduling of multipurpose batch processes: resource constraints and mixed storage policies." Ind. Eng. Chem. Res. 2005, 44, 426.
(37) Giannelos, N. F.; Georgiadis, M. C. A simple new continuous-time formulation for shortterm scheduling of multipurpose batch processes. Ind. Eng. Chem. Res. 2002, 41, 2178.
(38) Maravelias, C. T.; Grossmann, I. E. A hybrid MILP/CP decomposition approach for the continuous time scheduling of multipurpose batch plants. Comput. Chem. Eng. 2004, 28, 1921.
(39) Brooke, A.; Kendrick, D.; Meeraus, A.; Raman, R. GAMS: A user's guide; GAMS Development Corporation: South San Francisco, CA, 2003.


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