Planning and Scheduling of Flexible Process Networks Under Uncertainty with Stochastic Inventory: MINLP Models and Algorithm

Dajun Yue and Fengqi You
Dept. of Chemical and Biological Engineering, Northwestern University, Evanston, IL 60208

DOI 10.1002/aic.13924
Published online October 9, 2012 in Wiley Online Library (wileyonlinelibrary.com).

The tactical planning and scheduling of chemical process networks consisting of both dedicated and flexible processes under demand and supply uncertainty is addressed. To integrate the stochastic inventory control decisions with the production planning and scheduling, a mixed-integer nonlinear programming (MINLP) model is proposed that captures the stochastic nature of the demand variations and supply delays using the guaranteed-service approach. The model takes into account multiple tradeoffs and simultaneously determines the optimal selection of production schemes, purchase amounts of raw materials, sales of final products, production levels of processes, detailed cyclic production schedules for flexible processes, and working inventory and safety stock levels of all chemicals involved in the process network. To globally optimize the resulting nonconvex MINLP problems with modest computational times, the model properties are exploited and a tailored branch-and-refine algorithm based on the successive piecewise linear approximation is proposed. To handle the degeneracy of alternative optima in assignment configurations of production scheduling, three symmetry breaking cuts are further developed to accelerate the solution process. The application of the model and the performance of the proposed algorithm are illustrated through three examples with up to 25 chemicals and 16 processes including at most 8 production schemes for each flexible process. © 2012 American Institute of Chemical Engineers *AIChE J,* 59: 1511–1532, 2013
Keywords: planning, cyclic scheduling, stochastic inventory, MINLP, symmetry breaking cuts, advanced manufacturing

Introduction

Due to the increasing pressure for chemical companies to remain competitive in the global marketplace, enterprise-wide optimization (EWO) has become a major goal in the process industries.[1,2] As an opportunity for EWO, large integrated chemical complexes are constructed by chemical manufacturers around the world.[3] However, the tactical and operational decision making for various activities involved in such integrated chemical complexes is never trivial.[4] These chemical complexes involve diversified products and many interconnected processes, thus allowing the chemical production to take advantage of the synergies between processes.[5–7] Also, to ensure the flexibility of an integrated chemical complex, usually both dedicated and flexible processes are used, thus requiring the coordination among multiple production schemes.[8–11] In addition, the risks associated with demand variations and supply delays may significantly affect the decision making of a chemical complex.[12–14] Although inventories can serve as buffers in dealing with the demand and supply uncertainty, excessive inventory can be costly.[15,16] Moreover, as a large number of chemicals (raw materials, intermediates, and final products) are involved in a chemical complex, optimally determining which chemicals to be stored and their corresponding working and safety inventory levels is also a great challenge.[17,18] Generally, the production targets set at the planning level would affect the scheduling, and the production delays determined at the scheduling level would influence the lead times, thus having impacts on the inventory levels. As a chemical complex exhibits multiple tradeoffs among variables from all decision levels, it is of significant importance to develop a novel optimization framework that seamlessly integrates the planning, scheduling, and stochastic inventory management under demand and supply uncertainty.

The objective of this work is to propose a novel framework for the simultaneous optimization of midterm planning, scheduling, and stochastic inventory decisions for continuous flexible process networks. We propose an integrated model to coordinate the various decisions involved in a chemical complex, including the procurement of raw materials, production profiles of intermediate and final products, selection and scheduling of alternative production schemes, sales of final products to external markets, as well as the working inventory and safety stock levels of all chemicals under demand and supply uncertainty. We use the cyclic scheduling policy[8,9,19] to divide the entire planning horizon into several identical cycles, thereby establishing a bridge between different temporal scales. During each production cycle, we use the time slot formulation[11,20] to address the assignment of alternative production schemes in flexible processes. As a

Additional Supporting Information may be found in the online version of this article.

Correspondence concerning this article should be addressed to F. You at you@northwestern.edu.

chemical complex actually serves as a localized multiechelon supply chain,[3] we apply the stochastic inventory theory[15,16] to model the inventory system across the entire chemical complex. Using the guaranteed-service approach (GSA),[21–24] we are able to capture the stochastic nature of the supply and demand uncertainty and formulate an equivalent deterministic optimization model. The objective is to minimize the total cost, including the feedstock purchase costs, production operating costs, transition costs between different schemes and the inventory holding costs, meanwhile to satisfy the internal and external demands at a certain service level in a timely manner. We first formulate the model as a nonconvex mixed-integer nonlinear programming (MINLP) problem. To globally optimize the resulting MINLP with a modest computational time, we reformulate the model by taking advantage of the model properties and propose a tailored branch-and-refine algorithm based on the successive piecewise linear approximation. Furthermore, we develop three symmetry breaking cuts to eliminate the degeneracy of alternative optima in assignment configurations of production scheduling, which significantly accelerate the solution process. Three examples, with up to 25 chemicals and 16 processes including at most 8 production schemes for each flexible process, are presented to illustrate the application of the model and the performance of the proposed algorithm.

The novelties of this work are summarized as follows:

- Simultaneous optimization of midterm planning, scheduling, and stochastic inventory decisions for flexible process networks.
- A novel solution framework consisting of general linearization techniques, piecewise linear approximation, and integer cuts based on model properties.
- Efficient symmetry breaking cuts addressing the degeneracy in the assignment configuration for the scheduling of flexible processes.

The remaining article is organized as follows. In the next section, we review existing literature closely related to this work. In the "Background" section, we introduce some basics about the GSA and base-stock policy. The general "Problem Statement" is provided next, followed by the nonconvex MINLP model presented in the "MINLP Model Formulation" section. Then, an "Illustrative Example" is presented to illustrate the application of the proposed model. To solve large-scale problems, general linearization methods, a tailored branch-and-refine algorithm and three problem-specific integer cuts are presented in the "Solution Strategies" section. In the "Case Study" section, we present the computational results and discussion for two example problems. The "Conclusion" is given at the end of the article.

Literature Review

Our work falls into the category of the integration of planning and scheduling under uncertainty, which has drawn significant attentions in the past decade, and is still an active research area nowadays. General reviews on this topic are provided by Maravelias and Sung[4] and by Verderame et al.[25] The former focused on deterministic contributions, whereas the latter emphasized on uncertainty analysis.

Sahinidis and Grossmann[10] first proposed a multiperiod planning model for process networks with dedicated and flexible plants. Both continuous and batch operations are taken into consideration. Norton and Grossmann[5] extended the model by incorporating raw material flexibility in addition to product flexibility and provided a prototype of the chemical-process representation with alternative production schemes. Traditionally, planning and scheduling problems were treated separately. The scheduling problem was solved afterward to satisfy the production targets obtained from the planning problem.[26] This hierarchical approach may not necessarily lead to feasible schedules or global optimal solutions. Therefore, a number of simultaneous planning and scheduling models for multiproduct plants were proposed. Erdirik-Dogan and Grossmann[11] used a rigorous bilevel decomposition algorithm to reduce the computational cost and proposed integer and logic cuts to reduce the feasible search space for binary variables. Kopanos et al.[7] combined a discrete-time planning grid with a continuous-time treatment of the scheduling decisions considering product families. Sahinidis and Grossmann[9] and Pinto and Grossmann[8] applied cyclic scheduling policy and reformulated the model with linearization techniques and used generalized Benders decomposition and outer-approximation methods, respectively.

In the recent years, due to the highly dynamic global market environment, the integration of uncertainty analysis with planning and scheduling optimization models draws more and more attention. A classification of sources of uncertainty both inside and outside of a chemical complex was presented by Pistikopoulos,[14] among which, the demand variations and supply delays are mostly studied. The most common approach for optimization under uncertainty is the scenario-based two-stage stochastic programming.[27] Ierapetritou et al.[12] took advantage of the "value of perfect information" to transform stochastic models into "pseudodeterministic" equivalents. Liu and Sahinidis[13] used Monte Carlo sampling to estimate the expectation of the objective function, which facilitate the solution of large-scale problems. Ahmed and Sahinidis[28] introduced a robustness measure to account for the variability of the second-stage costs. Levis and Papageorgiou[29] considered clinical trials uncertainty when dealing with multisite capacity planning problems in the pharmaceutical industry based on the previous work by Papageorgiou et al.[30] Apart from the classic stochastic programming approach, You and Grossmann[31] introduced chance constraint programming when considering the design of responsive supply chains under demand uncertainty. Li et al.[32] explicitly considered demand due date and demand amount uncertainty at the operational planning level using a robust optimization approach.

Another body of research related to this work is the stochastic inventory theory, which can be traced back to the works by Simpson[33] and by Clark and Scarf[34] in the 1960s. It has been extensively studied by the Operations Research community and has quite a few applications in the supply chain management in the chemical industry. The main idea of stochastic inventory theory is using safety stocks as a means to deal with demand and supply uncertainty. At the beginning, its scope of application was limited to single-stage and sequential supply chains. Later, the stochastic inventory theory was extended to address general networks and became a powerful tool widely implemented in the supply chain management.[18,19,31,35–38] Contributions to multiechelon inventory optimization can be classified as either stochastic- or guaranteed-service framework.[21,39] A detailed comparison is presented by Klosterhalfen and Minner.[40] Here, we briefly state the distinguishing difference between these two approaches. In stochastic-service approach, the lead time is fixed, but the service level is stochastic. On the

contrary, in GSA, the service level is fixed, but the lead time is uncertain, which evolves into the service time. Although the stochastic inventory theory is originally developed for supply chain management, its application is not merely restricted in this area. You and Grossmann[17] introduced the stochastic inventory theory and GSA to study the tactical planning problem for chemical process networks. In their work, the optimal working and safety inventory levels for each chemical are explicitly optimized, and a tailored branch-and-refine algorithm was proposed to facilitate the solution process. However, only dedicated processes are considered in their work, and no scheduling issues were addressed.

Despite the significant developments in the relevant areas, to the best of our knowledge, in the existing literature, there is no modeling framework that integrates the stochastic inventory management with the planning and scheduling for flexible chemical process networks under the presence of demand and supply uncertainty, which is to be addressed in this work.

Background

In this section, we briefly review some concepts of GSA, which is used in this work to model the multiechelon stochastic inventory system across the entire chemical complex. For detailed discussion, one can refer to the works by Graves and Willems[21] and by You and Grossmann.[36]

In GSA, each stage or node in the multiechelon inventory system quotes a service time to its direct successor. This service is assumed to be guaranteed as long as the demand from its successor is within a certain upper bound. This upper bound is related to the service level specified at that node and the probability distribution of the uncertain demand. Service level stands for the probability or the frequency that demands can be satisfied, thus one minus the service level is the probability of stock-out.[15] The higher the service level is, the lower the risk of stock-out should be, thus the more safety inventories we need to hold. Therefore, the service level has a significant influence on the safety inventory levels, although it is considered as a given parameter in this work. If the demand exceeds its upper bound, we assume that the additional demand would be covered by special methods such as over time and/or expedited production.[23] Instead of explicitly modeling a tradeoff between possible shortage costs and inventory holding costs, the GSA treats the problem as being how to place safety stocks across a chemical complex to provide guaranteed service for the assumed bounded demand with the least inventory holding cost. This is reasonable, because it is often difficult in practice to assess shortage costs, and the notion of guaranteed service is somehow straightforward.[23] In summary, the main idea of the GSA is that the service level for each node in the multiechelon inventory system is fixed, but the service time is stochastic, which would have a direct impact on the optimal inventory level at each stockpoint.

With the aid of Figure 1, we would like to explain the stochastic timing relations in GSA. There are four major elements involved in the timing relationship of a multiechelon inventory system: the worst-case replenishment lead time of a node (T), the guaranteed service time (GST) a node quotes to its successor (S), the net lead time between two nodes (N), and the processing time from the gate of a node's predecessor to its own gate (P). The processing time can be

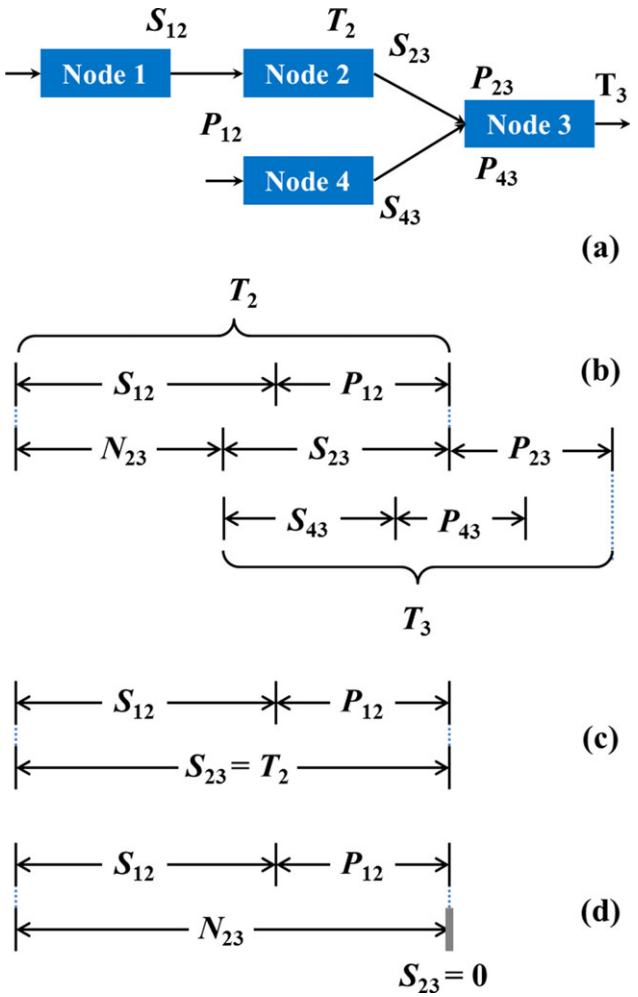

Figure 1. Stochastic timing relations in GSA.

(a) Multiechelon tree with four nodes, (b) part of timing relations at Nodes 2 and 3, (c) extreme case when the GST equals to the worst-case replenishment lead time (pull system), and (d) extreme case when the GST equals zero (push system). [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

further divided into the review period, the transportation time between two adjacent nodes and the production delay of the node. Figure 1a shows a simple multiechelon tree with timing elements marked next to the corresponding node. As Figure 1b suggests, once a node (Node 2) places an order to its predecessor (Node 1), after a certain GST (S_{12}), the order is guaranteed to arrive at this node (Node 2). Hence, the longest time that one has to wait until this node gets ready to service its successor (T_2) is equal to the sum of the GST (S_{12}) and the processing time (P_{12}). As the order from its successor (say Node 3) need not to be satisfied immediately but within a certain GST (S_{23}), the safety stock at this node is only required to cover demand variations over the net lead time (N_{23}). Note that if a node has multiple predecessors (Node 3), the worst-case replenishment lead time (T_3) takes the value of the maximum one, that is, $T_3 = \max\{S_{23} + P_{23}, S_{43} + P_{43}\}$. This is why it is called "worst case." There are two extreme cases in this timing relationship. As shown in Figure 1c, if the GST of a node to its successor is equal to its worst-case replenishment lead time, this node operates in "pull" mode. No safety inventory

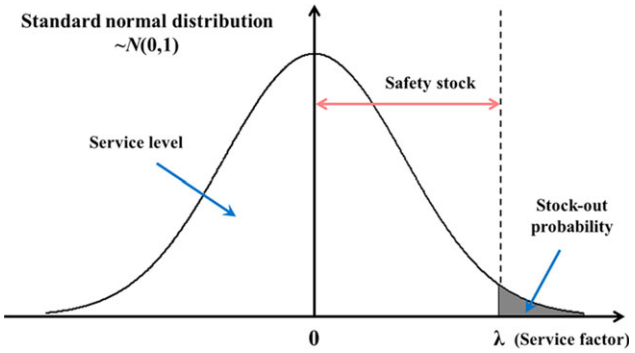

Figure 2. Standard normal distribution.

The white area between the curve and horizontal axis stands for the service level. The gray area between the curve and horizontal axis stands for the probability of stock out. The quantity between 0 and λ indicates the safety inventory level. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

is required in this case, and the net lead time equals to zero. On the other hand, as shown in Figure 1d, if the GST of a node to its successor is equal to zero, this node operates in "push" mode. The node holds the most safety stock in this case, and the net lead time equals to its worst-case replenishment lead time.

In GSA, each node is operating under a base-stock policy, with a common review period across the entire inventory system in the chemical complex. Under base-stock policy, the inventory level is reviewed on a regular basis (at the end of every day, every hour, etc.). At the same time when one checks the inventory level, a replenishment order is placed to bring the "inventory position" up to the base-stock level, where inventory position equals to inventory on-hand plus inventory in-transit. In this way, the replenishment amount or order quantity is equal to the difference between the current inventory position and the base-stock level. In this work, we assume the common review period is one day, and demands from external markets are satisfied also on a daily basis. If the daily demand of a node follows a normal distribution with mean μ and standard deviation σ (note that the unit of both μ and σ is ton/day), it is assumed that demand over any time interval is also normally distributed. Therefore, the total uncertain demand (say D_t) over the net lead time of N days follows $\mathbf{N}(N \cdot \mu, N \cdot \sigma^2)$ (note that actually N is dimensionless, which means the "number" of days). Recall that each stockpoint quotes a service level α to its downstream, which relates to the range of demand to be covered by the inventory system. Based on the previous discussion, it is obvious that the quantity $z = (D_t - N \cdot \mu)/\sigma\sqrt{N}$ follows standard normal distribution $\mathbf{N}(0,1)$ as shown in Figure 2.[15] By introducing the safety factor λ, which is a standard normal deviate for the service level α: $\Pr(z \leq \lambda) = \alpha$, we can derive the upper bound of the total demand over the net lead time, which is also the base-stock level, $BS = N\mu + \lambda\sigma\sqrt{N}$. This yields the safety stock for this stockpoint as $SS = \lambda\sigma\sqrt{N}$. In addition, the average on-hand inventory level is estimated as half of the expected demand (average working or cycle inventory) plus the safety inventory: $Inv. = N\mu/2 + \lambda\sigma\sqrt{N}$, which stands for the average inventory hold at the stockpoint.[41,42]

Problem Statement

In this work, we address the tactical planning and scheduling of chemical process networks consisting of both dedicated and flexible processes over a midterm planning horizon, meanwhile considering the demand and supply uncertainty through the use of stochastic inventory system. A general problem statement is given as follows.

As shown in Figure 3, given is a superstructure network consisting of a set of continuous processes $i \in I$, either dedicated $i \in DE$ or flexible $i \in FL$, a set of chemicals $j \in J$, a set of external suppliers $k \in K$, as well as a set of external markets $l \in L$. For each dedicated process, there is only one production scheme, whereas for each flexible process a set of production schemes $s \in S_i$ are specified. Note that the selections of production schemes are part of the planning-level decisions. We use the cyclic scheduling policy and slot-based formulation to coordinate the sequence and processing times of different production schemes in each flexible process. All the cycles of a process are identical, but different processes may have different cycles, of which the cycle time, production sequence, and scheme assignments are decision variables to be optimized. We also assume that all the processes are in use over the entire planning horizon, and the capacities of all processes are given. Chemicals can be raw materials, intermediates or products that may be purchased from external suppliers, produced/consumed by processes in the network, or sold to external markets. We use the GSA to capture the stochastic nature of the problem. The uncertainties of demand are hedged against by the safety inventories, and we assume that the daily demand for every product follows a normal distribution with the mean and standard deviation given by forecasts. The uncertainties of supplies are described in terms of GSTs from external suppliers and the availability of each chemical is known.

The objective is to minimize the total cost over the entire planning horizon, which consists of the purchase costs for raw materials from suppliers, the operating costs for all processes, the transition costs for flexible processes, and the inventory holding costs for all chemicals. To satisfy the demands in a timely manner at a minimum cost, the problem then involves determining the production profile of each process, the purchase and sale amount for every chemical, and the working inventory and safety stock levels of every chemical as well as the detailed cyclic schedule for each flexible process.

MINLP Model Formulation

A chemical-process network representation is used to account for the interactions between various chemical states and processes, as shown in Figure 3.[17] This representation is modified from the state-task network[43] and would greatly facilitate the analysis and modeling of the complex interactions between stochastic inventory management and the purchase, production, and sale activities. Chemicals are indicated by red circles with labels inside, which can be physically interpreted as storage tanks of chemicals. Processes are represented by blue boxes also with labels inside. Specifically, for flexible processes, the box is divided into several sublevels, each representing a production scheme. The external suppliers and markets are denoted by green boxes, respectively, on the left- and right-hand sides of the figure. In fact, this chemical-process network can be treated as a localized supply chain, involving various activities like

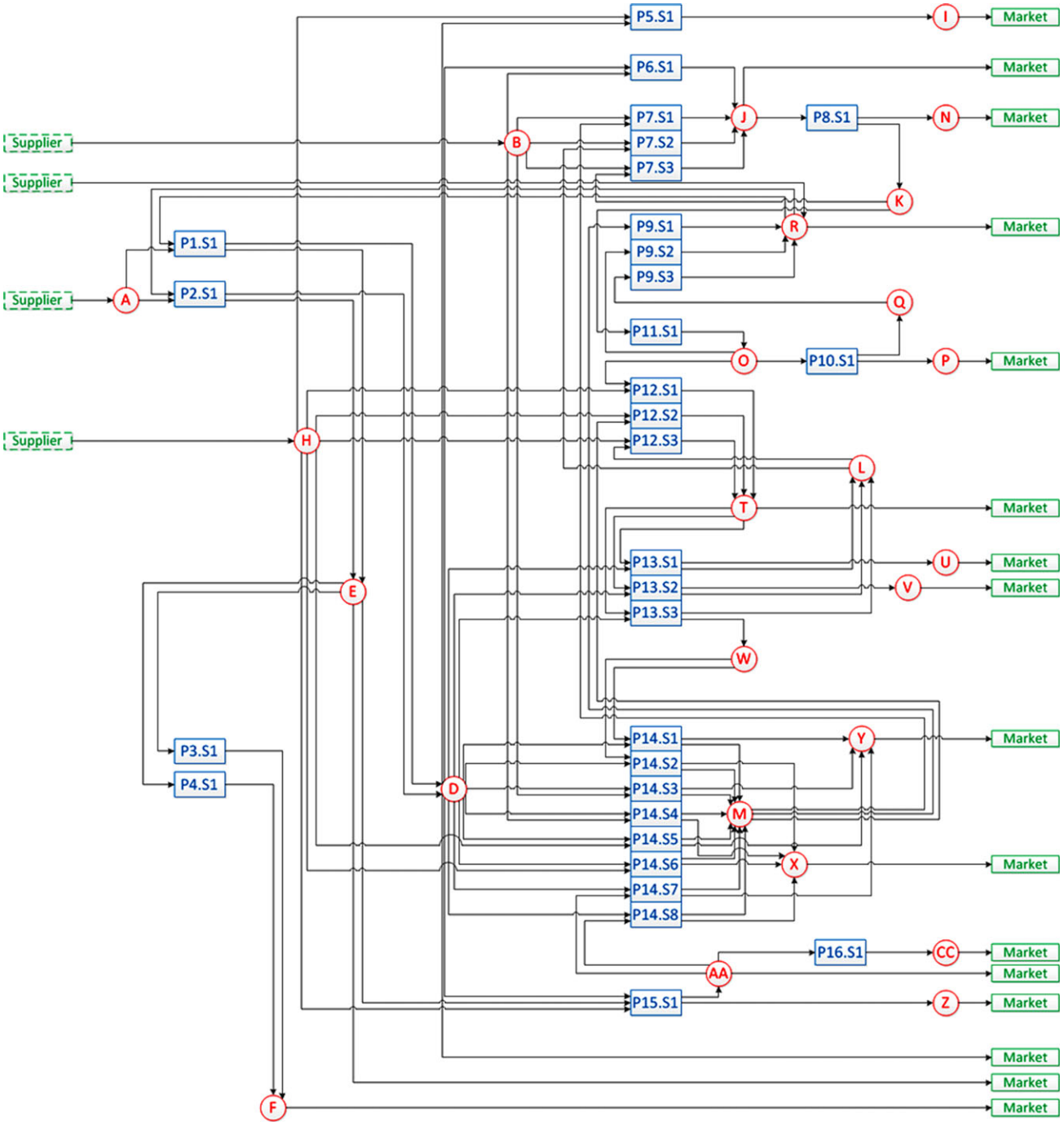

Figure 3. Chemical-process network representation of a chemical complex.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

procurement of raw materials, sale of final products, production of intermediate and final products, and storage of various chemicals across the chemical complex.

To simultaneously optimize the decisions from all levels, we first propose a nonconvex MINLP model, of which the model formulation is presented in the following sections. The objective is to minimize the total cost over the entire planning horizon, which is given by Eq. 32. The constraints can be classified into mass balance constraints 1–4, cyclic scheduling constraints 5–12, production planning constraints 13–15, stochastic timing constraints 16–24, internal demand constraints 25–28, and non-negative and integrity constraints 29–31. For convenience and clarity, we denote all the variables with upper case words, whereas parameters are in lower-case words. For further information, a list of sets/indices, parameters, and variables can be found in "Notation."

Mass balance constraints

For every chemical j, the total input including the amounts purchased from external suppliers and produced from upstream processes should be equal to the total output, including the amounts sold to external markets and consumed by downstream processes. Note that we consider only one period in this model, so the inventory is not included in

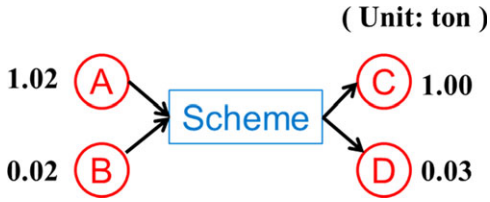

Figure 4. Linear material balance relationship for a production scheme.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

the overall mass balance constraint. We generally assume that the inventory levels at the end of the planning horizon are the same as their initial values. This overall mass balance relationship is given by the following constraint

$$\sum_{k\in SUP_j} PU_{j,k} + \sum_{(i,s)\in O_j} W_{i,s,j} = \sum_{(i,s)\in I_j} W_{i,s,j} + \sum_{l\in MKT_j} SA_{j,l}, \quad \forall j \tag{1}$$

where $PU_{j,k}$ is the amount of chemical j purchased from external supplier k, $SA_{j,l}$ is the amount sold to external market l, and $W_{i,s,j}$ is the amount produced/consumed by scheme s in process i. There are some subsets mentioned here. SUP_j is the subset of suppliers that provide chemical j. MKT_j is the subset of markets that have demand for chemical j. O_j is the subset of production schemes that produce chemical j, whereas I_j consumes chemical j.

If supplier k is selected to supply chemical j, the purchase amount should lie between the given lower bound $a^L_{j,k}$ and upper bound $a^U_{j,k}$; otherwise the purchase amount should be zero. This relationship is given by

$$a^L_{j,k}X_{j,k} \le PU_{j,k} \le a^U_{j,k}X_{j,k}, \quad \forall j,k \in SUP_j \tag{2}$$

where $X_{j,k}$ is a binary variable, which equals to 1 if there is positive flow from external supplier k to chemical j.

The expected sale amount of any chemical j to external markets l needs to satisfy the mean value of the demand over the planning horizon, which is the same as in the deterministic process planning. The demand variations will be handled by the base-stock policy and safety stocks. This relationship is given by

$$SA_{j,l} \ge \bar{\mu}_{j,l}h, \quad \forall j,l \in MKT_j \tag{3}$$

where $\bar{\mu}_{j,l}$ is the mean of demand rates and h is the planning horizon.

All chemical flows ($j \in C_{i,s}$) associated with production scheme s in process i are given by their material balance coefficient $\eta_{i,s,j}$ with respect to the main product ($j \in M_{i,s}$), which is positive for inputs and negative for outputs. For clarity, we provide an example in Figure 4, omitting subscripts s and i. Here, chemical C is the main product, thus chemical C belongs to set M, and all the chemicals A–D belong to set C. To produce 1 ton of chemical C, this scheme needs to consume 1.02 ton of chemical A and 0.02 ton of chemical B, and yields 0.03 ton of chemical D. Hence, $\eta_A = 1.02$, $\eta_B = 0.02$, $\eta_C = -1$, $\eta_D = -0.03$. The total mass of the inputs is always greater than or equal to that of the outputs, with the mass loss accounting for the byproducts, emissions, etc. Therefore, the linear material balance relationship is given by

$$W_{i,s,j} = |\eta_{i,s,j}|W_{i,s,j'}, \quad \forall i,s \in S_i, j \in C_{i,s}, j' \in M_{i,s} \tag{4}$$

Cyclic scheduling constraints

To coordinate the alternative production schemes in flexible processes, we consider the cyclic scheduling policy. Under this policy, the sequences and processing times of different schemes are determined together with the cycle time, and then the identical schedule is repeated over the entire planning horizon (Figure 5). During each cycle, using the slot-based formulation, the cycle time is divided into a number of time slots ($sl \in SL_i$), of which the number is equal to the number of available schemes in that flexible process. Each slot is further divided into a transition period and a processing period. For example, if a flexible process is able to perform four production schemes, each of its cycle contains four time slots (Figure 6). Then, the scheduling problem becomes how to assign the production schemes to the time slots.

The assignment constraint states that each time slot must be assigned to exactly one production scheme, whereas the same scheme can be assigned to more than one time slot. This relationship is given by

$$\sum_{s\in S_i} SY_{i,s,sl} = 1, \quad \forall i \in FL, sl \in SL_i \tag{5}$$

where $SY_{i,s,sl}$ is a binary variable, which equals to 1 if scheme s is assigned to slot sl in process i.

The sequence constraints state that the transition from scheme s' to scheme s occurs at the beginning of time slot sl if and only if scheme s is assigned to slot sl and scheme s' is assigned to the previous slot. Note that the transition variables $Z_{i,s,s',sl}$ can be treated as continuous variables between 0 and 1, instead of binary variables.[41] The proof is also provided in the Appendix. This significantly reduces the number of discrete variables and improves the computational efficiency.

$$\sum_{s\in S_i} Z_{i,s,s',sl} = SY_{i,s',sl-1}, \quad \forall i \in FL, s' \in S_i, sl \in SL_i \tag{6}$$

$$\sum_{s'\in S_i} Z_{i,s,s',sl} = SY_{i,s,sl}, \quad \forall i \in FL, s \in S_i, sl \in SL_i \tag{7}$$

$$0 \le Z_{i,s,s',sl} \le 1, \quad \forall i \in FL, s, s', sl \tag{8}$$

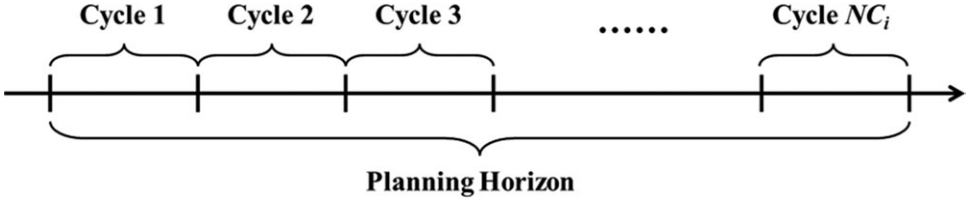

Figure 5. Cyclic scheduling policy.

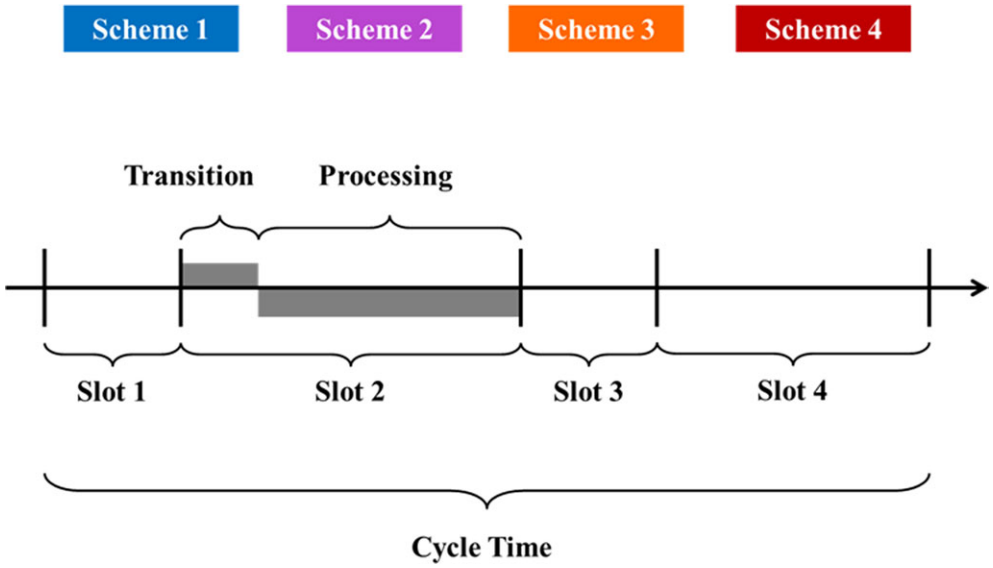

Figure 6. Time slot formulation for the scheduling of flexible processes.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

The cycle time CT_i is equal to the summation of transition times and production times in all the time slots, which is given by

$$CT_i = \sum_{sl \in SL_i} \sum_{s \in S_i} \Gamma_{i,s,sl} + \sum_{s \in S_i} \sum_{s' \in S_i} \sum_{sl \in SL_i} Z_{i,s,s',sl} \tau_{i,s,s'}, \quad \forall i \in FL \tag{9}$$

where $\Gamma_{i,s,sl}$ is the production time of scheme s in time slot sl in process i; $\tau_{i,s,s'}$ is the transition time from scheme s' to scheme s in process i.

As we assume that the processes are always in use over the entire planning horizon, the cycle time CT_i times the number of cycles NC_i for every flexible process should be equal to the length of the planning horizon. This yields the following equation

$$CT_i \cdot NC_i = h, \quad \forall i \in FL \tag{10}$$

If production scheme s is not assigned to time slot sl in process i, the corresponding production will not take place.

$$\Gamma_{i,s,sl} \le h \cdot SY_{i,s,sl}, \quad \forall i \in FL, s \in S_i, sl \in SL_i \tag{11}$$

The production level of each production scheme is measured in terms of its main product. For flexible processes, several production schemes may share the same process capacity. Thus, it requires that the production level of each scheme s in process i should not exceed the process capacity q_i. As the main products of different schemes may differ in density and other properties, the relative capacity factor $\rho_{i,s}$ is introduced.

$$W^S_{i,s,j} \le \sum_{sl \in SL_i} \rho_{i,s} q_i \Gamma_{i,s,sl}, \quad \forall i \in FL, s \in S_i, j \in M_{i,s} \tag{12}$$

where $W^S_{i,s,j}$ is the amount produced in a cycle.

Production planning constraints

For flexible processes, the total production amount over the planning horizon should be equal to the amount produced in a cycle times the number of cycles.

$$W^S_{i,s,j} NC_i = W_{i,s,j}, \quad \forall i \in FL, s \in S_i, j \in M_{i,s} \tag{13}$$

For dedicated processes, as there is only one production scheme, cyclic scheduling is not required. Therefore, the capacity constraint for dedicated processes is given by

$$W_{i,s,j} \le \rho_{i,s} q_i h, \quad \forall i \in DE, s \in S_i, j \in M_{i,s} \tag{14}$$

If production scheme s in process i is not selected, the production amount of the main product of this scheme should be zero.

$$W_{i,s,j} \le w^U_{i,s,j} YOP_{i,s}, \quad \forall i \in FL, s \in S_i, j \in M_{i,s} \tag{15}$$

where $w^U_{i,s,j}$ is the upper bound of the total production amount; $YOP_{i,s}$ is a binary variable, which equals to 1 if scheme s in process i is selected.

Stochastic timing constraints

A chemical complex can be treated as a multiechelon inventory system with both chemical nodes and process nodes. All the process nodes do not hold any inventories and operate in pull mode with zero net lead times. Inventories are only to be held at chemical nodes. In this work, we use the GSA to model the stochastic inventory system, assuming the service levels of all chemical nodes are known but the lead times are variables. Thus, the stochastic inventory model is based on the timing relationships among all chemical nodes and process nodes within the process network.

If scheme s in process i uses chemical j as one of the inputs, the worst-case replenishment lead time ($TP_{i,s}$) of this scheme should be no less than the sum of the GST ($SC_{i,j}$) and transfer time ($\theta_{i,j}$) from the storage tank of chemical j to this process plus the production delay ($PD_{i,s}$) of scheme s.

$$TP_{i,s} \ge SC_{i,j} + \theta_{i,j} + PD_{i,s}, \quad \forall j, (i,s) \in I_j \tag{16}$$

Note that there is no scheme index s in $SC_{i,j}$ or $\theta_{i,j}$. The GST and transfer time of chemical j to different schemes in

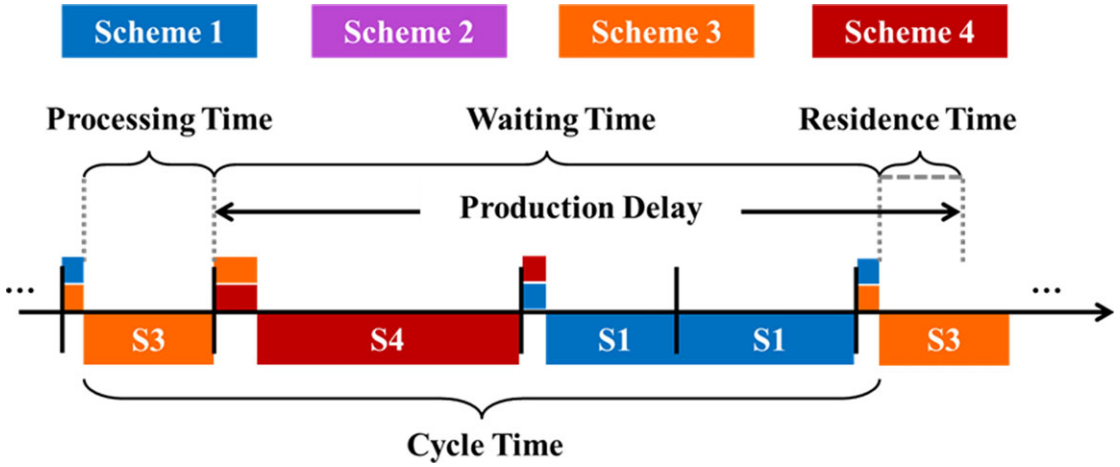

Figure 7. Production delay for flexible processes under cyclic scheduling policy.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

the same process should be the same, because they are in the same process.

As process nodes do not hold inventory, the net lead times are zero. Therefore, if chemical j is the product of scheme s, the GSTs ($SP_{i,s,j}$) to chemical j equals to the worst-case replenishment lead time of scheme s. Note that if a scheme has multiple products, the GSTs of all its products are the same, because they are produced at the same time.

$$SP_{i,s,j} = TP_{i,s}, \quad \forall j, (i,s) \in O_j \tag{17}$$

For dedicated processes, the production delay ($PD_{i,s}$) of scheme s in process i is simply its residence time

$$PD_{i,s} \geq \omega_{i,s}, \quad \forall i \in DE, s \in S_i \tag{18}$$

However, the production delays of flexible processes are more complicated to model due to the cyclic scheduling policy. For flexible processes, the inventory is a function of net lead time, which relates to the cycle time, processing time, and production delays of cyclic scheduling through constraint 19. Thus, we implicitly consider the inventory through the timing balance of cyclic scheduling and do not include it in the mass balance. As illustrated in Figure 7, the worst case is that one will need to adjust the production level of scheme s (say, S3) immediately after its completion. In this case, one will have to wait until scheme s (S3) is performed again. Thus, the time delay of scheme s is defined as the cycle time of process i plus its residence time minus its processing time.[19]

$$PD_{i,s} \geq CT_i + \omega_{i,s} - \sum_{sl \in SL_i} \Gamma_{i,s,sl}, \quad \forall i \in FL, s \in S_i \tag{19}$$

Note that if a flexible process is operating in "dedicated" mode, or in other words only one production scheme is selected in the process, constraint 19 downgrades to constraint 18, because the transition time to the scheme itself is zero, and the cycle time equals to the production time in this case.

Similarly, if chemical j is produced from production scheme s, the worst-case replenishment lead time (TC_j) of a chemical node j should be no less than the GST of scheme s plus the transfer time $\delta_{i,j}$. Otherwise, if there is no positive flow from scheme s to chemical node j, the worst-case lead time of chemical j would not be influenced by this scheme due to the activation of the big-M term.

$$TC_j \geq SP_{i,s,j} + \delta_{i,j} - M(1 - YOP_{i,s,t}), \quad \forall j, (i,s) \in O_j \tag{20}$$

where we can use the planning horizon h as the big-M parameter.

If some of chemical j is purchased from external supplier k, the worst-case replenishment lead time of chemical j should also be no less than the service time of this external supplier $si_{j,k}$. Note that the model allows the existence of multiple suppliers. One supplier can offer multiple chemicals and a chemical can be provided by different suppliers.

$$TC_j \geq si_{j,k} X_{j,k}, \quad \forall j, k \in SUP_j \tag{21}$$

where $X_{j,k}$ is a binary variable, which equals to 1 if there is positive flow from external supplier k to chemical node j.

If chemical j is consumed by scheme s, the GST of chemical j to its downstream production scheme s should be no less than the difference between the worst-case replenishment lead time of chemical j and the net lead time ($N_{i,j}$) of chemical j for the demand from process i.

$$SC_{i,j} \geq TC_j - N_{i,j}, \quad \forall j, i \in IP_j \tag{22}$$

If chemical j is sold to external market l, the GST of chemical j to this market ($SO_{j,l}$) should be no less than the difference between the worst-case replenishment lead time of chemical j and the net lead time ($\bar{N}_{j,l}$) of chemical j for the demand from market l.

$$SO_{j,l} \geq TC_j - \bar{N}_{j,l}, \quad \forall j, l \in MKT_j \tag{23}$$

In addition, the GST of chemical j to external market l should not exceed the maximum GST allowed by that market. Note that the model allows the existence of multiple markets. One market can have the demand for multiple chemicals, and a chemical can be consumed by multiple markets.

$$SO_{j,l} \le so^{U}_{j,l}, \quad \forall j, l \in MKT_j \tag{24}$$

Internal demand quantification

Because the demand of each final product from external markets is uncertain, the amount of each feedstock consumed by each production scheme in each process is also uncertain. As the external demands follow a normal distribution, these internal demands are also normally distributed. To determine the variance of an internal demand, we consider the variance-to-mean (VTM) ratio, which is the same for all the input chemicals of a certain production scheme. One can refer to the work by You and Grossmann[17] for further discussion on the internal demand quantification.

The variance of the internal demand ($V_{i,s,j}$) is given by

$$V_{i,s,j} = RP_{i,s} W_{i,s,j}/h, \quad \forall j, (i,s) \in I_j \tag{25}$$

where $RP_{i,s}$ is VTM ratio for all inputs of scheme s in process i.

There are two approaches to model the uncertainty propagation within the network: the ideal case and the worst case.[17] The ideal case suggests that the uncertainty propagation maintains the conservation of variance. However, in most cases, the level of uncertainty amplifies as the information flow transfers from downstream to upstream. Also, the latter case gives a more conservative inventory and tends to be computationally less expensive. Therefore, in this work, we only consider the worst case that is modeled by the following constraints

$$RC_j \ge RP_{i,s}, \quad \forall j, (i,s) \in I_j \tag{26}$$

$$RC_j \ge \bar{r}_{j,l}, \quad \forall j, l \in MKT_j \tag{27}$$

$$RP_{i,s} \ge RC_j, \quad \forall j, (i,s) \in O_j \tag{28}$$

where RC_j is the VTM ratio for all inputs of chemical j; $\bar{r}_{j,l}$ is the VTM ratio for the demand of chemical j from external market l.

It is worth mentioning that the above constraints may lead to an overestimation of the exact VTM ratios, thus causing a more conservative safety inventory. This is because not all the production schemes will be selected in the optimal process network structure. If a production scheme is not selected, the VTM ratios will not be propagated through it from downstream to upstream. Therefore, the inventory levels might be too conservative when the differences between VTM ratios of various external demands are considerable and the flexibility of the process network is significant. However, if one wants to model the exact uncertainty propagation within the network, a number of binary variables and big-M constraints need to be introduced. Moreover, the VTM ratios cannot be calculated a priori anymore (see "Uncertainty Propagation" in "Solution Strategies" section) and the bilinear term in Eq. 25 cannot be circumvented. Hence, to maintain the computational efficiency of the model, we still consider the relaxed formulation in our model.

Non-negative and integrity constraints

All the continuous variables in the model are non-negative. Binary variables should be either 1 or 0. Integer variables can take the values of 0, 1, 2…

$$\begin{aligned} &PU_{j,k}, W_{i,s,j}, SA_{j,l}, Z_{i,s,s',sl}, \Gamma_{i,s,sl}, W^{S}_{i,s,j}, \\ &CT_i, TP_{i,s}, SC_{i,j}, PD_{i,s}, SP_{i,s,j}, TC_j, \\ &N_{i,j}, \bar{N}_{j,l}, SO_{j,l}, V_{i,s,j}, RP_{i,s}, RC_j, NS_i, NY_{i,s} \ge 0 \end{aligned} \tag{29}$$

$$X_{j,k}, SY_{i,s,sl}, YOP_{i,s} \in \{0,1\} \tag{30}$$

$$NC_i \in \{0,1,2,3,\ldots\} \tag{31}$$

Objective function

The objective is to minimize the total cost given by

$$\begin{aligned} \min \; & \sum_i \sum_{s \in S_i} \sum_{j \in M_{i,s}} \varphi_{i,s} W_{i,s,j} + \sum_j \sum_{k \in SUP_j} \alpha_{j,k} PU_{j,k} \\ & + \sum_{i \in FL_i} \sum_{s \in S_i} \sum_{s' \in S_i} \sum_{sl \in SL_i} \pi_{i,s,s'} Z_{i,s,s',sl} NC_i \\ & + \sum_j \frac{1}{2} \beta_j h \left(\sum_{l \in MKT_j} \bar{N}_{j,l} \bar{\mu}_{j,l} + \sum_{(i,s) \in I_j} N_{i,j} W_{i,s,j}/h \right) \\ & + \sum_j \beta_j h \lambda_j \sqrt{\sum_{l \in MKT_j} \bar{N}_{j,l} \bar{v}_{j,l} + \sum_{(i,s) \in I_j} N_{i,j} V_{i,s,j}} \end{aligned} \tag{32}$$

The first term represents the operating costs, where $\varphi_{i,s}$ is the operating cost for producing one unit of the main product of scheme s in process i. The second term denotes the purchase costs, where $\alpha_{j,k}$ is the unit purchase cost of chemical j. The third term stands for the transition costs, where $\pi_{i,s,s'}$ is the sequence-dependent transition cost from scheme s' to scheme s. As for each flexible process, there are NC_i identical cycles, we need to time the number of cycles here. The inventory costs consist of two parts, one for the average working inventory and the other for the safety stocks, which are denoted, respectively, by the fourth and fifth term in the objective function. β_j is the unit inventory holding cost of chemical j; λ_j is the safety stock factor of chemical j; $\bar{v}_{j,l}$ is the variance for the demand of chemical j from external market l.

Nonconvex MINLP model

The constraints and objective function discussed earlier yields a nonconvex MINLP model, which we denote as (P1). The model includes constraints 1–31 and objective function 32. As we can see, there are bilinear terms in constraints 10, 13, 25, and the third, fourth, and fifth term of the objective function 32. Moreover, the square root functions in the fifth term of the objective function make the objective function nonconvex.

Illustrative Example

Example 1

To illustrate the application of the full-space MINLP model (P1), we first consider a small-scale example with the process network structure given in Figure 8. It consists of only 1 flexible process with 2 schemes and 4 chemicals in total.

In this problem, we assume the safety stock factor λ_j for all the chemicals are the same and equal to 2.0537, corresponding to a service level of 98%. The planning horizon is 300 days. The capacity of the process is 200 ton/day. The relative capacity factors of both schemes are 1. The demand for chemical C3 from the market follows a normal

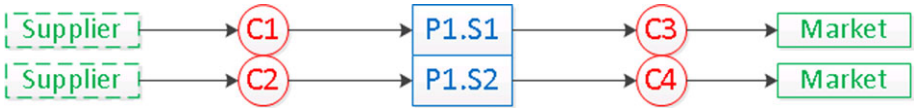

Figure 8. A single flexible process for Example 1.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

distribution with a mean of 100 ton/day and a standard deviation of 30 ton/day. The demand of chemical C4 from the market follows a normal distribution with a mean of 50 ton/day and a standard deviation of 20 ton/day. The maximum GSTs of chemical C3 and C4 to the market are fixed to zero. The deterministic transfer times from chemical node j to process i ($\theta_{i,j}$) and from process i to chemical node j ($\delta_{i,j}$) are neglected and set to zero. The supplier can provide unlimited raw materials C1 and C2 to the process with zero purchase lower bounds. Considering the length of the article, the remaining input data are given in Supporting Information.

The resulting MINLP model (P1) involves 9 discrete variables, 54 continuous variables, and 63 constraints. The problem size is rather small. To globally optimize the problem, we solve the problem with BARON 10.2.0[42] using GAMS 23.8.2.[44] After 36,000 s, the best solution returned suggests a total cost of \$10.56 million, with a gap of 11.2% between current lower and upper bounds. As can be seen, the global optimizer fail to converge to the global optimal solution even for this small-scale problem. Therefore, to handle large-scale problems, reformulation of the MINLP model and improvements in solution strategy are desired.

However, for this small-scale example, we can easily find out the assignment configuration. As chemical C3 is only produced from scheme S1 and chemical C4 only from scheme S2, both production schemes in the process must be selected. Because there are only two schemes, the sequence can be easily determined. We can fix the assignment variables $SY_{1,1,1} = 1$ and $SY_{1,2,2} = 1$, then solve the problem using BARON 10.2.0[42] again. This time, we obtain the optimal solution with 0% gap in less than 1 s. The minimum total cost suggested by the optimal solution is also \$10.56 million, which is the same as the one we got previously. This means that, although we can obtain the optimal solution in the early stage of the solution procedure, it fails to converge efficiently. This difficulty presumably arises from the selection of production schemes and the degeneracy of assignment configurations, and the solutions will be discussed in later sections.

The results for this example are presented as follows. The optimal cost profile is shown by the pie chart in Figure 9. The purchase cost account for the most (41%) of the total cost. The share of the inventory holding cost (30%) for this example is even larger than that of the production cost (24%). The transition cost accounts for the least (5%) of the total cost.

The optimal working inventory and cycle stock levels are shown in Figure 10. The working inventory levels for chemicals C1, C3, and C4 are 1020.0, 340.5, and 755.7 ton, respectively. The safety stocks held at the three chemical nodes are 196.8, 113.7, and 159.7 ton, respectively. However, we do not hold any inventory for chemical C2, thus node C2 is operating in pull mode with a zero net lead time to its downstream process.

The stochastic timing relationship is given as follows. As chemicals C1 and C2 are purchased from suppliers, the worst-case replenishment lead time of chemical C1 and C2 are equal to the GSTs of their corresponding suppliers, 10 days and 8 days, respectively. Chemical node C1 quotes a GST of 0 day to the process, thus the corresponding net lead time equals to 10 days. Chemical C2 quotes a GST of 8 days to the process, thus the corresponding net lead time equals to 0 day. The production delay of schemes S1 and S2 are 3.4 and 7.1 days, respectively. Therefore, the worst-case replenishment lead time of scheme S1, which also equals to its GSTs to downstream chemical nodes C3 and equals to the worst-case replenishment lead time of C3, is 3.4 days. As the maximum GST allowed by the market for C3 is 0 day, the net lead time at chemical node C3 is 3.4 days. Similarly, the net lead time at chemical node C4 is 15.1 days.

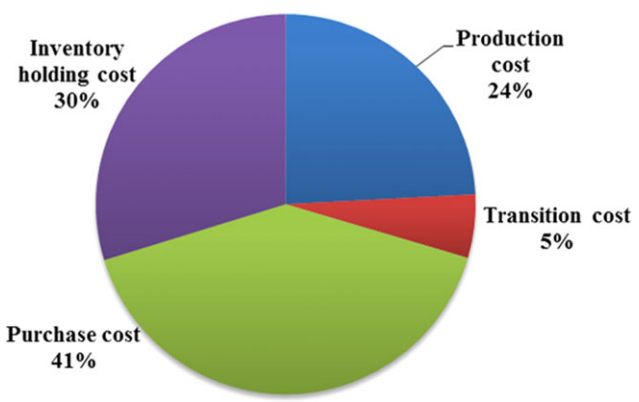

Figure 9. Optimal cost profile for Example 1.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

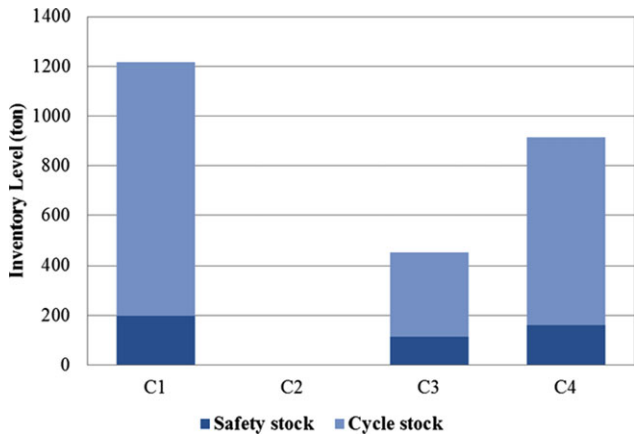

Figure 10. Optimal cycle and safety stock levels for Example 1.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Solution Strategies

In this section, we first exploit the model properties, and then apply general linearization techniques to reformulate the basic model into an MINLP, of which all the constraints are linear, and the only nonlinear terms are the square root functions in the objective function. Then, we propose a branch-and-refine algorithm based on successive piecewise linear approximation to globally optimize the reformulated model with a modest computational time. At last, we present three novel symmetry breaking cuts which significantly accelerate the solution process.

Uncertainty propagation

You and Grossmann[17] proposed that the optimal VTM ratios of internal demands can be predetermined based on the information of the process network. In other words, the variables RC_j and $RP_{i,s}$ can be treated as deterministic parameters during the optimization. This would significantly reduce the computational effort, because the bilinear terms in constraint 25 can then be replaced with linear functions.

The property is stated that the optimal VTM ratios of internal demands must be equal to one of the VTM ratios of the final demands $\bar{r}_{j,l}$. A path-search algorithm to determine the VTM ratios is also introduced in the same article. The major difference of the modified algorithm proposed below is that we explicitly model the uncertainty propagation through each production scheme in each process, because in addition to dedicated processes, flexible processes are considered in this work.

Step 1: Initialize $rp1_{i,s} = rp2_{i,s} = rc2_j = 0$, $diff = +\infty$; set $rc1_j = \max_{l \in MKT_j} \{\bar{r}_{j,l}\}$.

Step 2: $rp2_{i,s} = \max\{\max_j rc1_j, rp1_{i,s}\}$ for all i,s,j such that $(i,s) \in O_j$.

Step 3: $rc2_j = \max\{\max_{(i,s)} rp1_{i,s}, rc1_j\}$ for all i,s,j such that $(i,s) \in I_j$.

Step 4: $rc2_j = \max\{\max_{l \in MKT_j} \bar{r}_{j,l}, rc2_j\}$.

Step 5: Evaluate $diff = \sum_j (rc2_j - rc1_j)^2 + \sum_{(i,s)} (rp2_{i,s} - rp1_{i,s})^2$; set $rp1_{i,s} = rp2_{i,s}$, $rc1_j = rc2_j$.

Step 6: If $diff < 10^{-6}$, then set $RP^*_{i,s} = rp1_{i,s}$, $RC^*_j = rc1_j$ and stop; else go to Step 2 and iterate.

General linearization methods for bilinear terms

As suggested by Glover,[45] a bilinear term in the form as the product of a non-negative continuous variable and a binary variable can be linearized by introducing one auxiliary non-negative variable, one big-M parameter and three additional constraints. For example, the bilinear term $(B \cdot C)$ could be replace by a non-negative variable K by adding the following constraints

$$K \le C \tag{33}$$

$$K \le M \cdot B \tag{34}$$

$$K \ge C - M(1 - B) \tag{35}$$

where B is a binary 0–1 variable, C is an arbitrary non-negative continuous variable, and M is a sufficiently large parameter. If the binary variable B is zero, constraint 34 would force K to zero and constraint 35 becomes redundant; if B is one, constraint 33 indicates that $K \le C$, meanwhile constraint 35 suggests that $K \ge C$, which leads to $K = C$.

Furthermore, the bilinear term in the form as the product of a non-negative continuous variable and a non-negative integer variable can also be linearized in the same way by expressing the integer variable using a set of binary variables. For example, an arbitrary positive integer variable I can be expressed as follows

$$I = \sum_m 2^{|m|-1} \cdot B_m \tag{36}$$

where the binary variable B_m determines the value of the mth digit of the binary representation of I.[46]

We apply the binary representation to variables NC_i and $N_{i,j}$, which are given as follows

$$NC_i = \sum_{m \in M1} 2^{|m|-1} \cdot DN_{i,m}, \quad \forall i \in FL \tag{37}$$

$$N_{i,j} = \sum_{m \in M2} 2^{|m|-1} \cdot D_{i,j,m}, \quad \forall j, i \in IP_j \tag{38}$$

where $DN_{i,m}$ and $D_{i,j,m}$ are the binary variables for the mth digit of NC_i and $N_{i,j}$, respectively.

As the production delay is determined with the cyclic schedules, which could take fractional values, the net lead time $N_{i,j}$ is not necessarily an integer variable in this work. By rounding the net lead time $N_{i,j}$ to an integer, we indicate an overestimation of the objective function.

In this way, the bilinear terms in constraints 10, 13, and the third, fourth, and fifth term in the objective function 31 can be linearized using the Glover linearization scheme. Considering the length of the article, the Glover linearization constraints are omitted and the reformulated constraints are given in the following equations.

Constraint 10 is reformulated as follows

$$\sum_{m \in M1} 2^{|m|-1} DNCT_{i,m} = h, \quad \forall i \in FL \tag{39}$$

where $DNCT_{i,m}$ is the auxiliary variable for $(CT_i \cdot NC_i)$.

Constraint 13 is reformulated as follows

$$\sum_{m \in M1} 2^{|m|-1} DNWS_{i,s,j,m} = W_{i,s,j}, \quad \forall i \in FL, s \in S_i, j \in M_{i,s} \tag{40}$$

where $DNWS_{i,s,j,m}$ is the auxiliary variable for $(W^S_{i,s,j} \cdot NC_i)$.

For the purpose of concise expression in later derivations, we introduce two non-negative variables O_j and G_j as follows

$$O_j = \sum_{l \in MKT_j} \bar{N}_{j,l} \bar{\mu}_{j,l} + \sum_{m \in M2} \sum_{(i,s) \in I_j} 2^{|m|-1} DW_{i,s,j,m}/h, \quad \forall j \tag{41}$$

$$G_j = \sum_{l \in MKT_j} \bar{N}_{j,l} \bar{v}_{j,l} + \sum_{m \in M2} \sum_{(i,s) \in I_j} 2^{|m|-1} DV_{i,s,j,m}, \quad \forall j \tag{42}$$

where $DW_{i,s,j,m}$ and $DV_{i,s,j,m}$ are the auxiliary variables for $(N_{i,j} \cdot W_{i,s,j})$ and $(N_{i,j} \cdot V_{i,s,j})$, respectively.

Finally, the reformulated objective function becomes

$$\begin{aligned} \min \; & \sum_i \sum_{s \in S_i} \sum_{j \in M_{i,s}} \varphi_{i,s} W_{i,s,j} + \sum_j \sum_{k \in SUP_j} \alpha_{j,k} PU_{j,k} \\ & + \sum_{m \in M1} \sum_{i \in FL_i} \sum_{s \in S_i} \sum_{s' \in S_i} \sum_{sl \in SL_i} \pi_{i,s,s'} 2^{|m|-1} DNZ_{i,s,s',sl,m} \\ & + \sum_j \frac{1}{2} \beta_j h O_j + \sum_j \beta_j h \lambda_j \sqrt{G_j} \end{aligned} \tag{43}$$

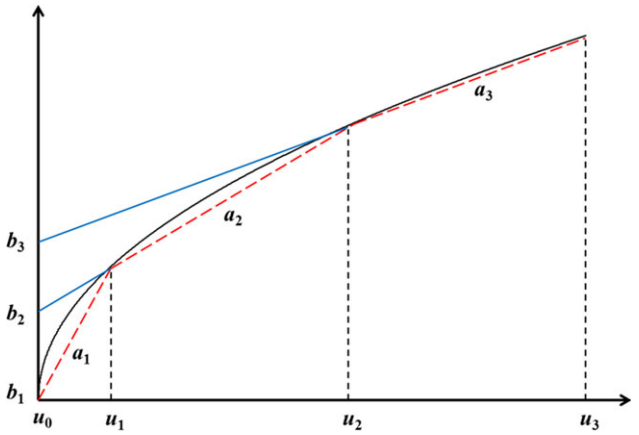

Figure 11. Piecewise linear approximation of a concave function.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

where $DNZ_{i,s,s',sl,m}$ is the auxiliary variable for $(Z_{i,s,s',sl} \cdot NC_i)$.

So far, we have derived a reformulated MINLP model, whose objective function is given by Eq. 43 and subject to constraints 1–9, 11, 12, 14–25, 29, 30, 37–42, and the omitted Glover linearization constraints. As can be seen, all the constraints are linear, and the only nonlinear terms in the model are the square root terms in the objective function.

Piecewise linear approximation

So far, after the reformulation and linearization, all the constraints are linearized. The only nonlinear terms in the model are the square root terms $\sqrt{G_j}$ in the objective function. As the square root function is concave, as shown in Figure 11, we consider a piecewise linear function (red dashed lines) as an underestimation of this nonlinear term (black solid curve) by using the "multiple-choice" formulation. Note that besides the multiple-choice model, substitutive formulations also include the incremental model and the convex combination model. In this work, we simply choose one out of the three.[47,48] Let $P_j = \{1, 2, 3, \ldots, p\}$ denotes the set of pieces or intervals in the piecewise linear function $f(G_j)$, and $u_{j,0}, u_{j,1}, u_{j,2}, \ldots, u_{j,p}$ be the lower and upper bounds of G_j for each interval. The multiple-choice formulation for every chemical j is given by

$$f(G_j) = \sum_{p \in P_j} (b_{j,p} E_{j,p} + a_{j,p} F_{j,p}), \quad \forall j \tag{44}$$

$$\sum_{p \in P_j} E_{j,p} = 1, \quad \forall j \tag{45}$$

$$\sum_{p \in P_j} F_{j,p} = G_j, \quad \forall j \tag{46}$$

$$u_{j,p-1} E_{j,p} \le F_{j,p} \le u_{j,p} E_{j,p}, \quad \forall j, p \in P_j \tag{47}$$

$$E_{j,p} \in \{0,1\}, \quad F_{j,p} \ge 0, \quad \forall j, p \in P_j \tag{48}$$

$$a_{j,p} = \frac{\sqrt{u_{j,p}} - \sqrt{u_{j,p-1}}}{u_{j,p} - u_{j,p-1}}, \quad b_{j,p} = \sqrt{u_{j,p}} - a_{j,p} u_{j,p}, \quad \forall j, p \in P_j \tag{49}$$

Replacing the square root function $\sqrt{G_j}$ in the objective function with the piecewise linear function $f(G_j)$ yields the following objective function

$$\begin{aligned} \min \; & \sum_i \sum_{s \in S_i} \sum_{j \in M_{i,s}} \varphi_{i,s} W_{i,s,j} + \sum_j \sum_{k \in SUP_j} \alpha_{j,k} PU_{j,k} \\ & + \sum_{m \in M1} \sum_{i \in FL_i} \sum_{s \in S_i} \sum_{s' \in S_i} \sum_{sl \in SL_i} \pi_{i,s,s'} 2^{|m|-1} DNZ_{i,s,s',sl,m} \\ & + \sum_j \frac{1}{2} \beta_j h O_j + \sum_j \beta_j h \lambda_j \sum_{p \in P_j} (b_{j,p} E_{j,p} + a_{j,p} F_{j,p}) \end{aligned} \tag{50}$$

Therefore, we have derived a mixed-integer linear programming (MILP) model (P2), which includes constraints 1–9, 11, 12, 14–25, 29, 30, 37–42, 45–49, and the objective function 50. As the signs before all square root functions in the Eq. 50 are positive, when they are replaced by the corresponding piecewise linear functions, Eq. 50 provides an underestimation of Eq. 43. Also, models (P1) and (P2) have the same feasible region, so they have the same set of feasible solutions. In the next section, we will present the algorithm that takes advantage of this MILP for the solution of the reformulated nonconvex MINLP.

Branch-and-refine algorithm

Because the objective of (P2) is an under-estimator of the objective of (P1) and this is a minimization problem, the optimal objective of (P2) provides a valid lower bound to the basic model (P1). As both models have the same feasible region, the optimal solution of (P2) is also a feasible solution of (P1). Therefore, we can always obtain an upper bound of the global optimal solution by directly substituting the optimal solution of (P2) to evaluate the objective function of (P1). The remaining challenge is how to iteratively refine and improve the solution, so that the gap between the lower and upper bounds will converge within finite iterations. Obviously, the more pieces that are used in (P2), the better the approximation we can get for the nonlinear function $\sqrt{G_j}$, but more additional variables and constraints are required. Instead, we consider an iterative branch-and-refine strategy starting from only one interval for each $f(G_j)$, and let the algorithm automatically determine whether additional intervals are needed or not.[17,35] The flowchart of this algorithm is illustrated in Figure 12. For a more detailed explanation, one can refer to the work by You and Grossmann.[17]

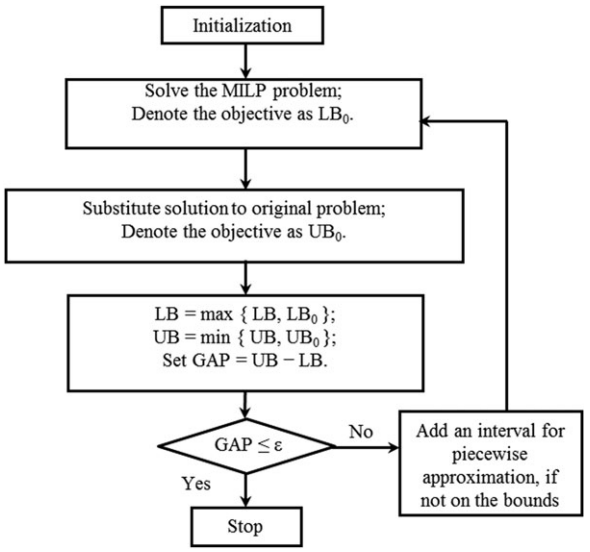

Figure 12. Flowchart of the branch-and-refine algorithm.

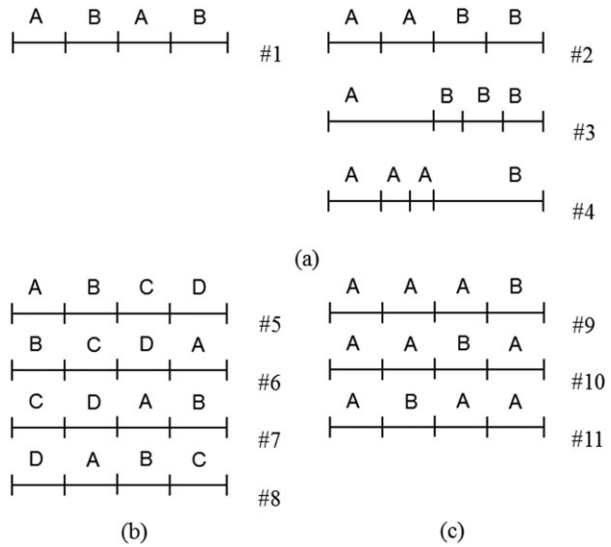

Figure 13. Degeneracy of assignment configurations in scheduling.

(a) A nonoptimal solution and degenerate configurations related to CUT 1, (b) Degenerate configurations related to CUT 2, and (c) Degenerate configurations related to CUT 3.

Symmetry breaking cuts

From observation, we discovered that the major computational difficulty arises from the selection and scheduling of production schemes in the flexible processes. This is mostly because that when the same product can be assigned to more than one slot, the cyclic scheduling model becomes highly degenerate. As suggested in the work by Erdirik-Dogan and Grossmann,[11] introducing symmetry breaking cuts could improve the computational efficiency of the model. When the same product is assigned to more than one slot, the model will not assign that product to nonconsecutive slots in the optimal solution. For example, Configuration 1 in Figure 13a results in the same production performance but higher transition cost compared to Configuration 2. However, Configurations 2–4 are all equivalent. To prevent these degenerate solutions, they enforced that if a selected scheme is not assigned to the first slot, it can only occupy exactly one slot and the scheme assigned to the first slot would utilize all the remaining slots (CUT 1). This is modeled by the following constraints

$$NY_{i,s} = \sum_{sl \in SL_i} SY_{i,s,sl}, \quad \forall i \in FL, s \in S_i \tag{51}$$

$$YOP_{i,s} \geq SY_{i,s,sl}, \quad \forall i \in FL, s \in S_i, sl \in SL_i \tag{52}$$

$$YOP_{i,s} \leq NY_{i,s} \leq nsl_i YOP_{i,s}, \quad \forall i \in FL, s \in S_i \tag{53}$$

$$NS_i = \sum_{s \in S_i} YOP_{i,s}, \quad \forall i \in FL \tag{54}$$

$$NY_{i,s} \geq nsl_i - (NS_i - 1) - M(1 - SY_{i,s,1}), \quad \forall i \in FL, s \in S_i \tag{55}$$

$$NY_{i,s} \leq nsl_i - (NS_i - 1) + M(1 - SY_{i,s,1}), \quad \forall i \in FL, s \in S_i \tag{56}$$

where $NY_{i,s}$ stands for the number of time slots assigned to scheme s in process i; NS_i represents the number of schemes that are selected in process i; nsl_i is the number of schemes or slots in process i. Constraints 51–54 are straightforward. CUT 1 mentioned before is enforced by the two big-M constraints 55 and 56. If a scheme is assigned to the first slot, the big-M terms in both constraints become zero, thus the number of slots assigned to this scheme must be equal to the total number of slots nsl_i, minus the total number of selected schemes minus 1. If the scheme is not assigned to the first slot, both constraints become redundant. As the number of slots assigned to a scheme will not exceed nsl_i. We can use nsl_i as the big-M parameter.

However, for cyclic scheduling, this symmetry breaking cut alone is not enough. As can be seen in Figure 13b, Configurations 5–8 are also equivalent. This indicates that as long as the mutual sequence of the production schemes remain unchanged, either one of them can be assigned to the first slot. Thus, we propose a new symmetry breaking cut enforcing that the scheme assigned to the first slot has the smallest order among all the selected schemes (CUT 2). To model this, we introduce an auxiliary variable $CUT_{i,s,s',sl}$ which equals to 1 if scheme s' is assigned to the first slot and scheme s to slot sl in process i. Similar to the transition variables $Z_{i,s,s',sl}$, $CUT_{i,s,s',sl}$ can be defined as continuous variables between 0 and 1, instead of binary variables.[41] CUT 2 is modeled by the following constraints

$$\sum_{s \in S_i} CUT_{i,s,s',sl} = SY_{i,s',1}, \quad \forall i \in FL, s' \in S_i, sl \in SL_i, |sl| > 1 \tag{57}$$

$$\sum_{s' \in S_i} CUT_{i,s,s',sl} = SY_{i,s,sl}, \quad \forall i \in FL, s \in S_i, sl \in SL_i, |sl| > 1 \tag{58}$$

$$CUT_{i,s,s',sl} = 0, \quad \forall i \in FL, s \in S_i, s' \in S_i, sl \in SL_i, |sl| > 1, |s| < |s'| \tag{59}$$

Note that $|sl| > 1$ indicates slots other than the one with the least order, and $|s| < |s'|$ indicates that the order of scheme s is smaller than that of s'.

Furthermore, as can be seen in Figure 13c, Configurations 9–11 satisfy both cuts mentioned earlier but are still alternative optima. Therefore, we propose another symmetry breaking cut (CUT 3) enforcing that if the scheme assigned to the first slot occupies more than one slot, then they must be the first few slots which can be modeled by

$$-M \cdot CUT_{i,s,s',sl} + 1 \leq |sl| - NY_{i,s'} \leq M \cdot (1 - CUT_{i,s,s',sl}), \quad \forall i \in FL, s \in S_i, s' \in S_i, |s| = |s'|, sl \in SL_i, |sl| > 1 \tag{60}$$

This big-M constraint states that if a scheme is simultaneously assigned to the first slot and slot sl other than the first slot, the big-M term on the right-hand side becomes zero, thus the order of slot sl cannot exceed the number of slots assigned to this scheme. If this is not the case, the constraint becomes redundant. As the number of slots assigned to a scheme will not exceed nsl_i, we can use nsl_i as the big-M parameter.

In this way, we are able to eliminate all the other degenerate assignment configurations in scheduling, except the one that satisfies all the three symmetry breaking constraint. Although this would introduce additional variables and constraints, it would greatly accelerate the computation process

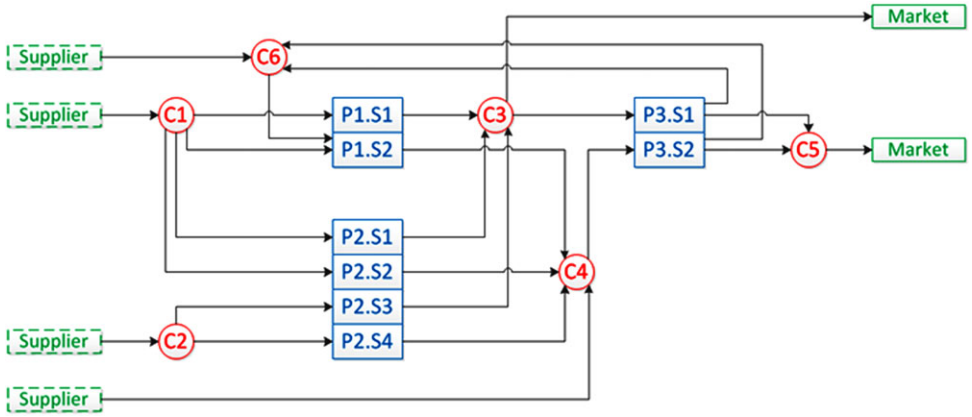

Figure 14. Process network superstructure for Example 2.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

due to the significant reduction in feasible search space. Comparison results will be presented in the next section.

Case Studies

To illustrate the application of the reformulated model and the performance of the proposed solution strategies, we consider a medium-scale problem (Example 2) and a large-scale chemical complex network (Example 3). All the computational experiments are performed on a DELL OPTIPLEX 790 desktop with Intel(R) Core(TM) i5-2400 CPU @ 3.10 GHz and 8 GB RAM. All the models and solution procedure are coded in GAMS 23.8.1.[44] The MILP problems are solved using CPLEX 12.4. The nonconvex MINLP problems are solved using BARON 10.2.0[42] to achieve global optimality.

Example 2

In this example, we consider a process network consisting of 6 chemicals and 3 flexible processes including at most 4 production schemes each, given by Figure 14. The planning horizon is 350 days. The safety stock factors are set to 2.0537 corresponding to a 98% service level. All the demands of chemicals from external markets are normally distributed. The purchase lower bounds, the maximum GSTs to markets and the deterministic transfer times between process nodes and chemical nodes are all set to zero. The remaining input data are given in Supporting Information.

For this example, we set the optimality tolerance for the solvers as 0%. We first solve the full-space problem with the basic nonconvex MINLP formulation (P1) using the solver BARON 10.2.0.[42] Unfortunately, no feasible solution is returned because of "solver failure" after 1,440 s. The solver failure might be due to the connection between the NLP solver CONOPT and the global optimizer BARON. Then, we solve the model (P2) that does not include the symmetry breaking cuts, using the proposed branch-and-refine algorithm with the solver CPLEX 12.4. It took 1,575 CPUs in total for three iterations of the branch-and-refine algorithm to achieve the global optimal solution with a zero optimality gap. This shows significant improvement in the computational efficiency using the reformulated model and the proposed branch-and-refine algorithm. At last, we add the three symmetry breaking cuts and solve the resulting model (P3) using CPLEX 12.4. This time, we obtain the same global optimal solution with only 376 CPUs in total for three iterations. The comparison shows that it is worth introducing the additional variables and constraints of the symmetry breaking cuts. The upper and lower bounds of each iteration of the proposed branch-and-refine algorithm when solving model (P3) are demonstrated in Figure 15. The algorithm finds the optimal solution at the first iteration and spends two more iterations to verify its optimality. However, this is not always the case. In general, the upper bound may

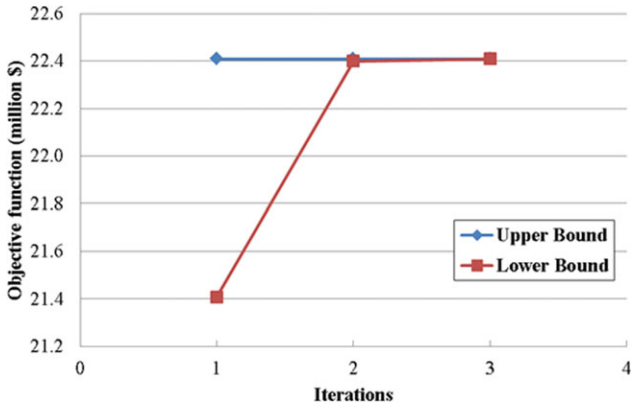

Figure 15. Upper and lower bounds of each iteration of the branch-and-refine algorithm for Example 2.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

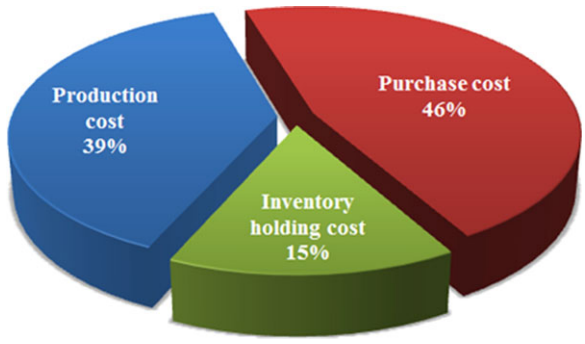

Figure 16. Cost profile for Example 2.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

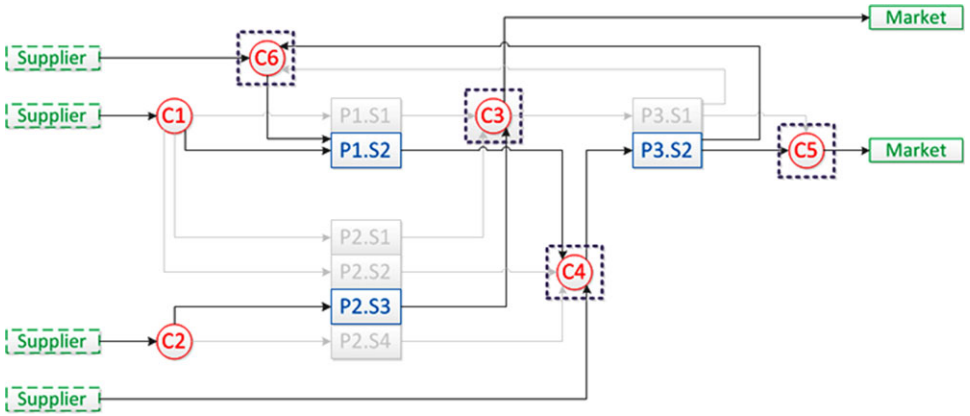

Figure 17. Optimal process network structure for Example 2.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

gradually decrease and lower bound increases as the number of iterations goes up.

The global minimum total cost obtained is $22.41 million with the profile shown in Figure 16. We can see that the purchase costs account for almost half of the total cost. The inventory holding cost represents 15% of the total cost, which significantly demonstrates the importance of integrating inventory optimization with process planning and scheduling decisions. The transition cost is zero, because there is no transition between different production schemes. As can be seen clearly in the optimal network structure shown in Figure 17, all three flexible processes are operating in dedicated mode with only one production scheme selected in each process.

The dash-line boxes indicate that the chemical being surrounded has a nonzero inventory level. Thus, in the optimal network structure we do not need to hold any inventory for chemicals C1 and C2. In order words, these two chemical nodes are operating in pull mode with zero net lead time. The optimal purchase and sale amounts are listed in Table 1. The demand for chemical C3 is fully satisfied by production scheme S3 in process P2 using chemical C2 purchased from external supplier as the feedstock. Chemical C5 is produced by scheme S2 in process P3 using chemical C4 as the input. Part of chemical C4 is purchased from the external supplier, whereas the other part is produced from scheme S2 in process P1 using chemical C1 and C6 as inputs. Note that chemical C6 is also the coproduct of chemical C5, thus forming a recycle stream in the process network. The optimal production level for each scheme is shown in Figure 18, which indicates that processes P1 and P2 are operating at their full capacity of 70 and 100 ton/day, respectively. However, process P3 only utilizes 70 out of 150 ton/day of the full capacity, leaving more than half of the capacity unused.

Figure 19 shows the stochastic timing relations within the chemical-process system. As can be seen, the optimal network can be divided into two subsystems. One involves processes P1 and P3 and chemicals C1, C4, C5, and C6. The other involves process P2 and chemicals C2 and C3. The former subsystem involves a recycle stream. The worst-case replenishment lead time of chemical C1 equals to the GST of its supplier, 10 days. Chemical node C1 operates in pull mode and quotes a GST of 10 days to scheme S2 in process P1. As the production delay of scheme S2 is 2 days, it quotes a GST of 12 days to chemical C4, which is coincidently equal to the GST from the supplier to chemical node C4. Thus, the worst-case replenishment lead time of chemical C4 is 12 days. Chemical C4 operates in push mode and quotes a GST of 0 day to scheme S2 in process P3. As the production delay of scheme S2 is 1 day, it quotes GST of 1 day to both its products C5 and C6. As part of chemical C6 is also purchased from the supplier that quotes a GST of 15 days, the worst-case replenishment lead time has to be 15 days. As an internal chemical, which would not be sold to the market, chemical C6 quotes a GST of 10 days back to scheme S2 in process P1, thus resulting in a net lead time of 5 days. The latter subsystem is a sequential network. The worst-case replenishment lead time of chemical C2 equals to GST of the supplier, 8 days. Chemical node C2 operates in pull mode and quotes a GST of 8 days to scheme S3 in process P2. As the production delay of scheme S3 is 2 days, it quotes GST of 10 days to chemical C3.

Table 1. Optimal Purchase and Sale Amounts for Example 2

Chemicals	Purchases $PU_{j,k}$ (ton)	Sales $SA_{j,l}$ (ton)
C1	26,950	
C2	37,800	
C3		35,000
C4	2450	
C5		24,500
C6	980	

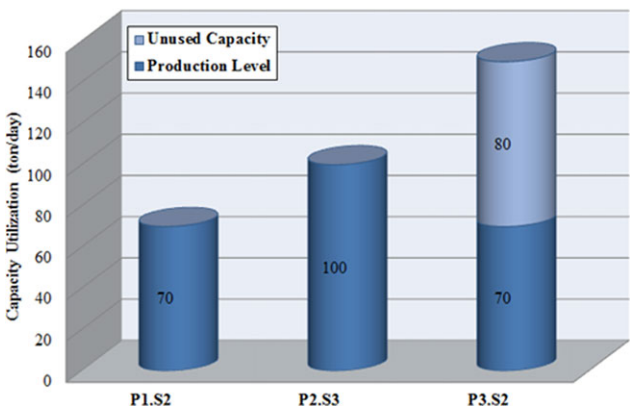

Figure 18. Optimal production levels and capacity utilization for Example 2.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

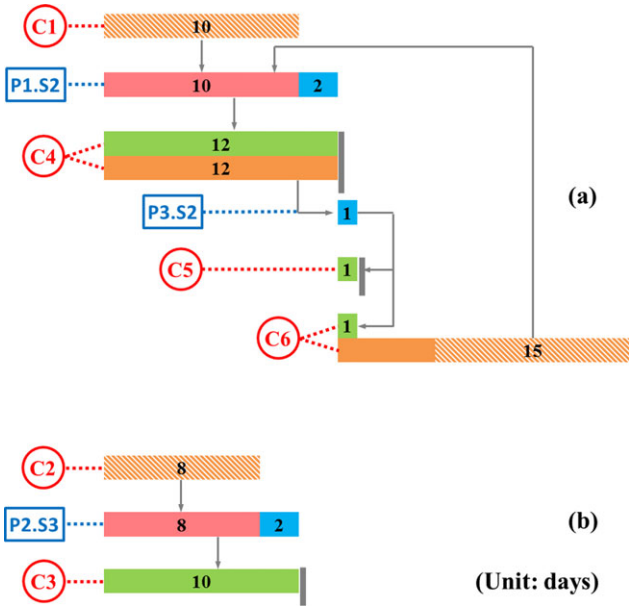

Figure 19. Stochastic timing relations for Example 2.

(a) Subsystem consisting of chemicals C1, C4, C5, and C6 and processes P1 and P3. (b) Subsystem consisting of chemicals C2 and C3 and process P2. Orange bars denote GSTs from external suppliers to chemical nodes. Portions with the slashed pattern and pink bars denote GSTs of chemical nodes to downstream processes. Blue bars denote production delays of processes. Green bars denote GSTs of processes to downstream chemical nodes. Vertical gray bars denote zero GSTs. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

The GSTs of chemical nodes that face external markets can be treated as a quantitative indicator of responsiveness, which measures the ability of a chemical complex to respond rapidly to changes in demand.[19,37] If we increase the maximum GSTs of the demands from the market, we will be able to achieve a lower total cost, because the demands are becoming less urgent. Thus, we perform a series of computational experiments by setting all the maximum GSTs $so_{j,l}^{U}$ to a same value and gradually increasing the value from 0 to 15. The results presented in Figure 20 shows that as the GSTs of the demands for chemicals from the external market increase from 0 to 15 days, the total cost monotonically decreases from \$22.4 million to \$19.3 million, and the total inventory for all chemicals drops from 2,492.7 to 45.6 ton. We have not plotted for the cases such that $so_{j,l}^{U} > 15$, because the total cost and inventory profile will not decrease anymore. The result shows that the more responsive the process network needs to be, the higher cost and more inventory it will have. The reason that the total inventory level of this example cannot reach zero will be discussed in the next paragraph.

Figure 21 shows the optimal working and safety inventory levels for all chemicals when the GSTs of demands from the market are set to 0, 5, 10, and 15 days, respectively. In addition to the decrease in inventory levels, the number of chemicals to be stored is also changing. For the case of 0 day, we hold inventories for four products, for the case of 5 days we store three products, and for the case of 10 days, we store two products. In the case of 15 days, we only need to hold inventory for one product, C6. The inventory of chemical C6 cannot reach zero, because chemical C6 is within a cycle stream. To explain this point, let us have a look at the instance illustrated in Figure 22. The notations of the parameters are the same as those in Figure 1. Assuming both N_{12} and N_{21} are 0, and $T_1 = S_{21} + P_{21}$, we can derive that $T_1 = S_{12}$ and $S_{12} + P_{12} = T_2 = S_{21}$, which leads to a contradictory result: $T_1 = P_{12} + P_{21} + T_1$. Therefore, in this case, at least one of the net lead times in the cycle stream must be non-negative, which would cause the inventory placement at this node.

Example 3

To illustrate the application of the proposed models and the performance of the branch-and-refine algorithm and symmetry breaking cuts on large-scale problems, recall the chemical-process network discussed at the beginning of the article (Figure 3). We still consider the same assumptions in Example 2, setting the purchase lower bounds, the maximum GSTs to markets and the deterministic transfer times between process nodes and chemical nodes to zero. The planning horizon is also 350 days. The detailed input data are given in Supporting Information.

Considering the large problem size, we set the optimality tolerance as 0.1%. We first solve the full-space problem (P1) using BARON 10.2.0.[42] After about 3,300 s, we encounter the solver failure again. We then solve (P2), which does not include the symmetry breaking cuts using the proposed branch-and-refine algorithm with CPLEX 12.4. The lower bounding problem of the first iteration in the branch-and-refine algorithm cannot converge to the solution with desired optimality tolerance after 36,000 s. At last, we solve (P3) that includes the symmetry breaking cuts with the proposed branch-and-refine algorithm using CPLEX 12.4. The global optimal solution is obtained within three iterations with a total CPU time of 5,926 s.

The optimal process network is shown in Figure 23. Note that the supplier of chemical R is not selected. All the internal and external demands of chemical R are satisfied by the production of process P9. Also note that the chemical node W is not selected. There are neither processes consuming/producing chemical W, nor external markets having demand for chemical W. Although in the original superstructure, some flexible process involves 8 production schemes, at most 2 schemes are chosen in the optimal network. The

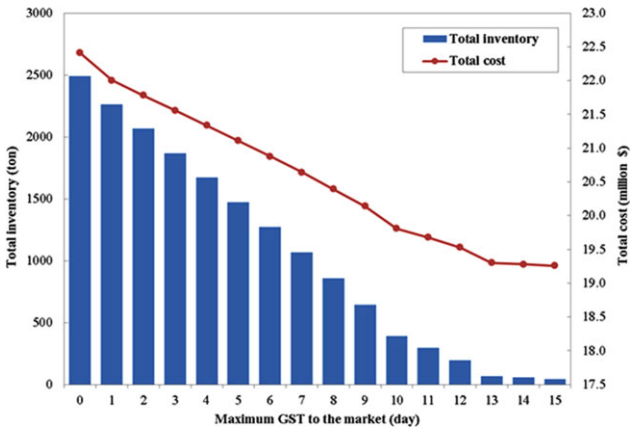

Figure 20. Pareto optimal curve and total inventory of all chemicals for Example 2.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

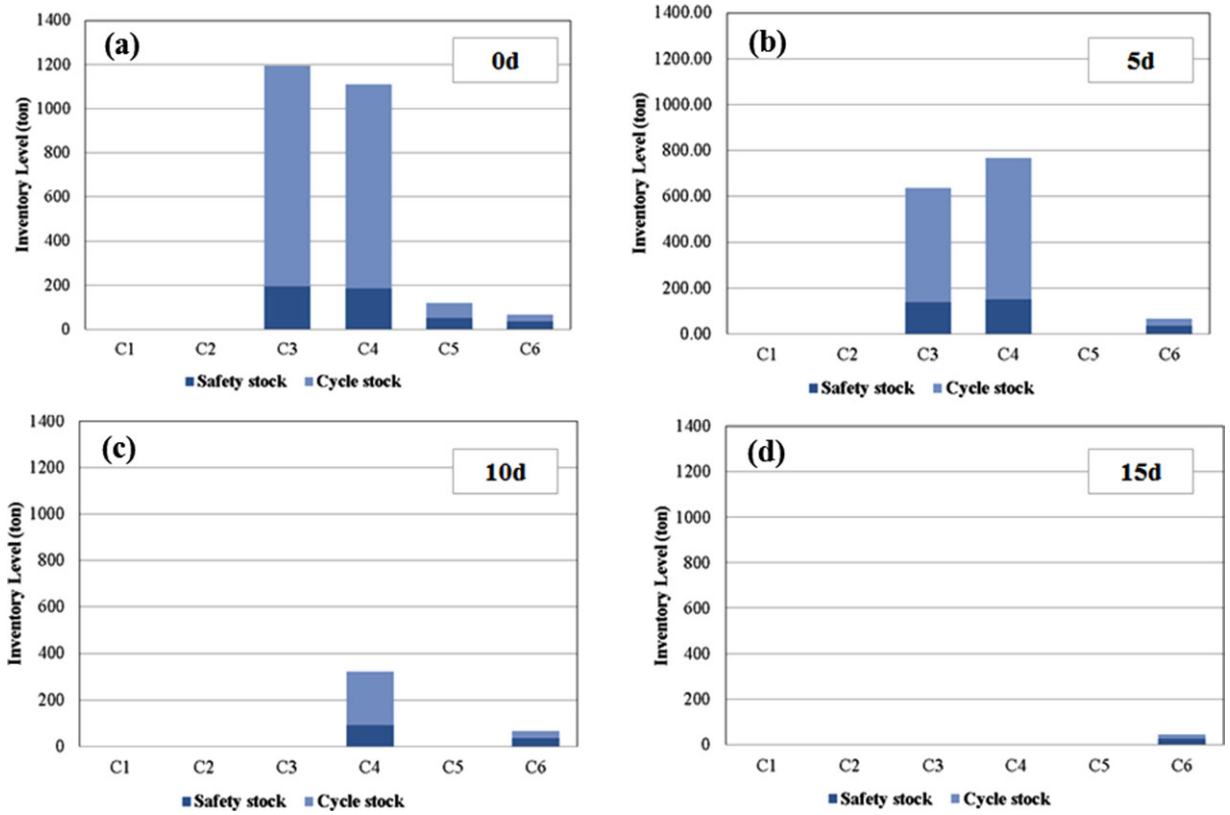

Figure 21. Optimal inventory levels when all the maximum GSTs to the market are set to different values.

(a) Case when maximum GSTs to the market are 0 day, (b) case when maximum GSTs to the market are 5 days, (c) case when maximum GSTs to the market are 10 days, and (d) case when maximum GSTs to the market are 15 days. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

cyclic schedules for flexible processes are presented in Table 2. As can be seen, the cycle times range from 1 to 3 weeks. Note that the summation of processing times of the chosen schemes is less than the cycle time of the flexible process, because transition times are not listed. Also, as only two schemes are chosen, the sequence can be easily determined under the cyclic scheduling policy.

The corresponding inventory profile is shown in Figure 24a. Some chemical nodes such as A, B, K, M, and O are operating in pull mode with zero net lead times and inventories. Some chemical nodes keep rather low inventory levels, whereas some others keep very high inventory levels. Especially, for chemical J, its inventory level is much higher than those of other chemicals. This is because the unit inventory holding cost for chemical J is much lower than other chemicals, and also because it is an important intermediate and final product.

To address the responsiveness issue of this chemical complex, we perform the same analysis as discussed in Example 2. This time we generate 24 instances by fixing the parameters $so^U_{j,l}$ to 24 values evenly distributed in [0, 69], that is, 0, 3, 6…66, 69. The resulting Pareto optimal curve is shown in Figure 25. As this is a minimization problem, a lower error bar for the total cost indicating the 0.1% optimality gap is considered for each instance. In general, as we increase the GSTs to the market from 0 to 69 days, the total cost drops from \$362.2 million to \$344.8 million, and the total inventory drops from 30,007 to 7,324 ton. As can be seen, the total cost as well as the total inventory level drops sharply as $so^U_{j,l}$ increases from 0 to 18 days, whereas tends to be flat after 27 days. Considering a balance between costs and responsiveness, one may set the GSTs to markets as 3 weeks, but any point on the Pareto curve is optimal. Theoretically, the total cost should be monotonically decreasing. However, slight fluctuations of the total cost can be observed in the lower-right part of the curve. The fluctuation of the total cost is because the model is solved with a 0.1% gap rather than the zero optimality tolerance. The same reason applies to the fluctuation of the total inventory level, whereas another reason is the existence of multiple optimal solutions due to the trade-off between stochastic inventory management and other activities involved in the chemical complex. Figure 24 shows the optimal working and safety inventory levels for all chemicals when the GSTs of demands from the market are set to 0, 15, 30, 45, 60, and 69 days. As can be seen, when the GSTs are set to 0 day, the optimal solution suggests holding inventory for 19 out of 25 chemicals. As we relax the maximum GSTs allowed by the market, the number of chemicals one needs to

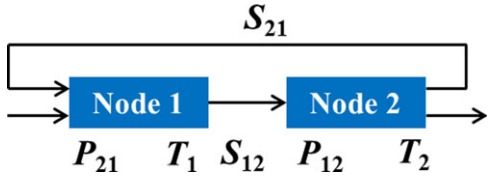

Figure 22. Illustration of stochastic timings in a cycle stream.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

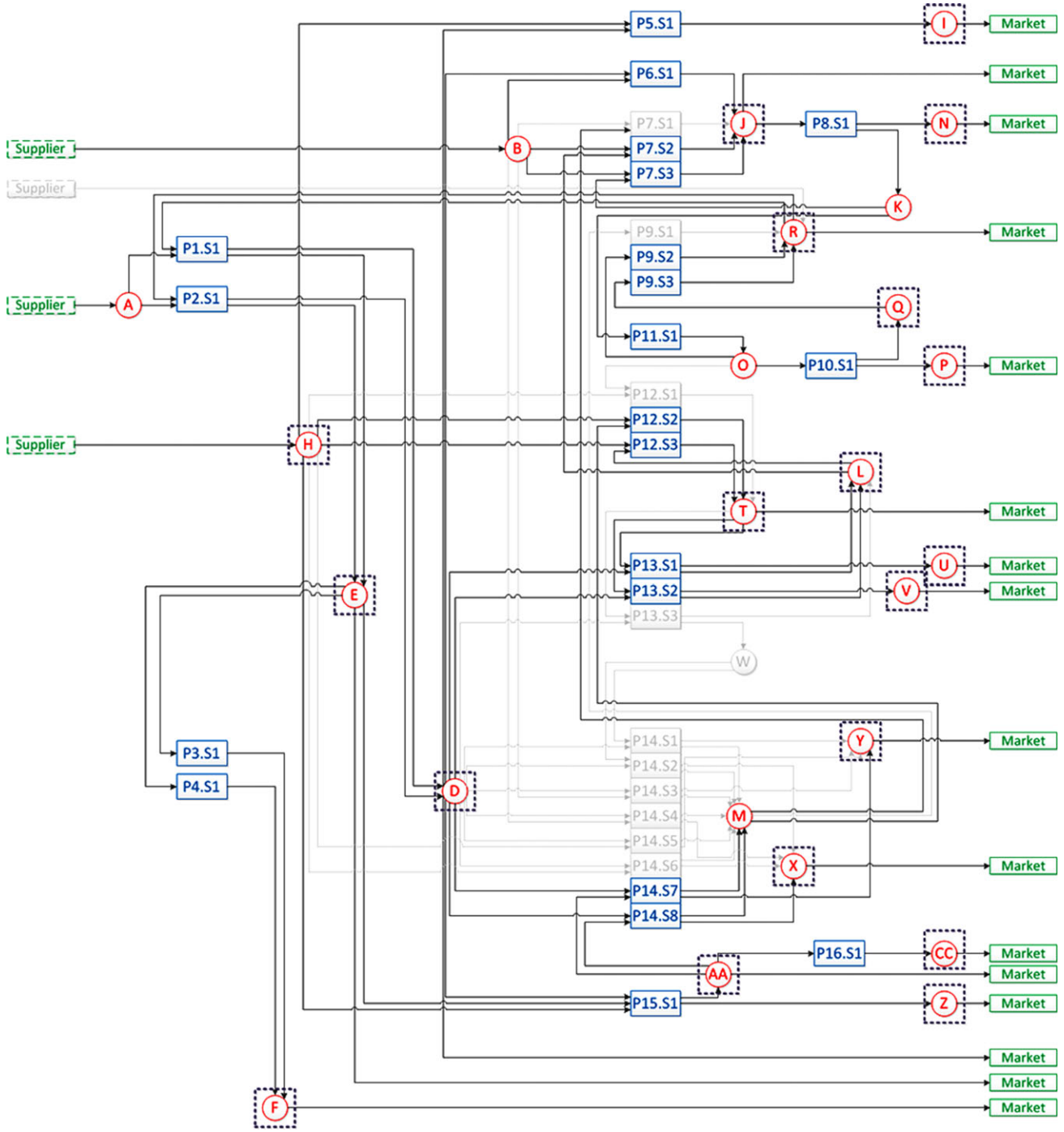

Figure 23. Optimal process network for Example 3.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

hold decreases. When the GSTs are set to 69 days, the optimal solution suggests holding inventory just for four important intermediate and final products. Although the total inventory decreases as the GSTs increase, the inventory level for a certain chemical may increase, for example, the inventory level of chemical R in Figures 24c,f. This is because the objective is to minimize the total cost rather than the inventory level of a certain chemical.

Conclusions

In this work, we addressed the integration of tactical planning, scheduling, and stochastic inventory management for

Table 2. Cyclic Schedules for Example 3

Process	Scheme	Processing Time (day)	Cycle Time (day)	Number of Cycles
7	2	16.0	19.4	18
	3	2.6		
9	2	10.9	18.4	19
	3	6.9		
12	2	5.2	10.3	34
	3	4.2		
13	1	4.8	8.0	44
	2	2.5		
14	7	2.8	8.8	40
	8	4.8		

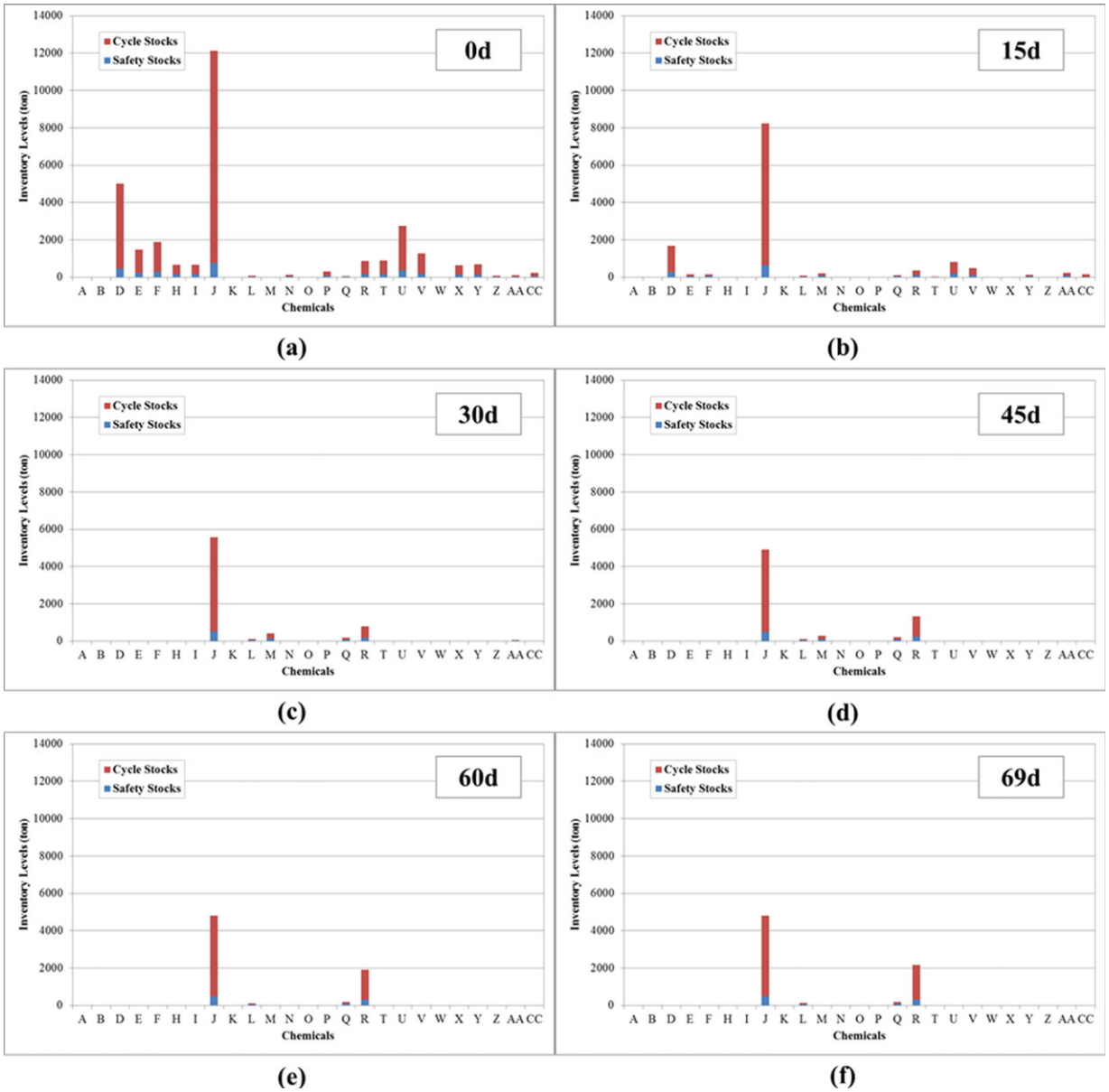

Figure 24. Optimal inventory levels when maximum GSTs to the market are set to different values.

(a) Case when maximum GSTs to the market are 0 day, (b) case when maximum GSTs to the market are 15 day, (c) case when maximum GSTs to the market are 30 day, (d) case when maximum GSTs to the market are 45 day, (e) case when maximum GSTs to the market are 60 day, and (f) case when maximum GSTs to the market are 69 day. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

chemical complexes, which include both dedicated and flexible processes, under supply and demand uncertainty. We used the GSA to capture the stochastic nature of demand variations and supply delays, and we used the cyclic scheduling policy to coordinate the processing of alternative production schemes. We proposed a nonconvex MINLP model that simultaneously determines the scheme selections, production schedules, purchases, sales, production/consumption amounts, and working and safety inventory levels. This model considered multiple tradeoffs among variables from all decision levels, thus seamlessly integrated the planning, scheduling, and stochastic inventory management. As this basic model contained multilinear and concave terms, which could be computationally intractable for large-size problems, we reformulated the model to an MINLP with only square root and linear terms by exploiting the problem properties and using general linearization methods. To obtain global optimal solutions with modest computational times, we further developed a tailored branch-and-refine algorithm based on successive piecewise linear approximations. Moreover, three novel symmetry breaking cuts were proposed to eliminate the degeneracy of the assignment configurations, which in turn greatly accelerated the computation. Three examples, with up to 25 chemicals and 16 processes including at most eight production schemes for each flexible process, were presented to illustrate the application of the model and its computational performance. The computational results showed that the proposed solution framework can reduce the computational times of solving the nonconvex MINLP by orders of magnitude. To examine the responsiveness issues of chemical complexes, we presented approximated Pareto-optimal curves to reveal the trade-offs between the total cost and

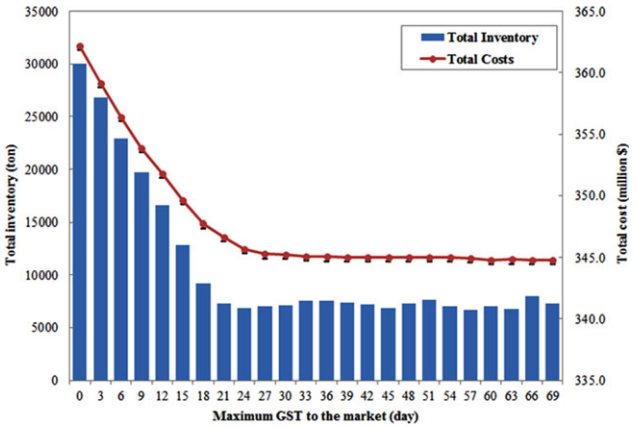

Figure 25. Pareto optimal curve and total inventory of all chemicals for Example 3.

Lower error bars are added for each instance on the Pareto curve, representing the 0.1% optimality gap. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

inventory vs. the maximum GSTs to the markets. The results show that the more responsive the process network needs to be, the higher cost and more inventory it will have.

Notation

Sets/indices

I = set of processes indexed by i
J = set of chemicals indexed by j
K = set of external suppliers indexed by k
L = set of external markets indexed by l
M = set of digits for binary representation indexed by sl
P = set of pieces for piecewise linear approximation indexed by p
S = set of production schemes indexed by s
SL = set of time slots indexed by sl

Subsets

$C_{i,s}$ = subset of chemicals j that are inputs or outputs of scheme s in process i
DE = subset of dedicated processes i
FL = subset of flexible processes i
I_j = subset of production schemes s in process i that consume chemical j
IP_j = subset of processes i that consume chemical j
$M_{i,s}$ = subset of chemical j that is the main product of schemes s in process i
MKT_j = subset of external markets l that have demand for chemical j
$M1$ = subset of digits m for binary representation of the numbers of cycles
$M2$ = subset of digits m for binary representation of the net lead times
O_j = subset of production schemes s in process i that produce chemical j
P_j = subset of pieces for piecewise linear approximation for chemical j
S_i = subset of production schemes s available in process i
SL_i = subset of time slots sl in process i
SUP_j = subset of external suppliers k that supply chemical j

Parameters

$a^L_{j,k}$ = lower bound for the availability of chemical j at external supplier k
$a^U_{j,k}$ = upper bound for the availability of chemical j at external supplier k
$a_{j,p}$ = tangents for piecewise linear approximation
$b_{j,p}$ = intercepts for piecewise linear approximation
h = planning horizon
nsl_i = number of time slots/production schemes in process i
q_i = production capacity of process i
$\bar{r}_{j,l}$ = variance-to-mean ratio for the demand for chemical j of external market l
$si_{j,k}$ = GST for chemical j from external supplier k
$so^U_{j,l}$ = maximum service time allowed for chemical j to external market l
$u_{j,p}$ = bounds of intervals for piecewise linear approximation
$v^U_{i,s,j}$ = upper bound of internal demand variance for chemical j of scheme s in process i
$\bar{v}_{j,l}$ = variance for the demand of chemical j of external market l
$w^U_{i,s,j}$ = upper bound for the amount of chemical j produced by scheme s in process i
$\alpha_{j,k}$ = unit purchase cost for chemical j from external supplier k
β_j = unit inventory holding cost of chemical j
$\delta_{i,j}$ = deterministic transfer time from process i to chemical j
$\eta_{i,s,j}$ = material balance coefficient of chemical j for scheme s in process i
$\theta_{i,j}$ = deterministic transfer time from chemical j to process i
λ_j = safety stock factor for chemical j
$\bar{\mu}_{j,l}$ = mean value of external demand for chemical j from market l
$\pi_{i,s,s'}$ = transition cost from scheme s' to s in process i
$\rho_{i,s}$ = relative capacity factor of main product of scheme s in process i
$\tau_{i,s,s'}$ = transition time from production scheme s' to$s$ in process i
$\varphi_{i,s}$ = unit operating cost for scheme s in process i
$\omega_{i,s}$ = residence time of scheme s in process i

Binary variables

$D_{i,j,m}$ = digit m for binary representation of net lead times of chemical j to process i
$DN_{i,m}$ = digit m for binary representation of number of cycles of process i
$E_{j,p}$ = auxiliary variable for piecewise linear approximation
$SY_{i,s,sl}$ = 1 if slot sl is assigned to scheme s in process i
$X_{j,k}$ = 1 if there is positive flow from external supplier k to chemical j
$YOP_{i,s}$ = 1 if scheme s in process i is selected

Non-negative integer variable

NC_i = number of cycles of process i

Non-negative continuous variables

CT_i = cycle time of process i
$CUT_{i,s,s',sl}$ = 1 if scheme s' is assigned to the first slot and scheme s to slot sl in process i
$DV_{i,s,j,m}$ = auxiliary variable for the linearization of bilinear terms
$DW_{i,s,j,m}$ = auxiliary variable for the linearization of bilinear terms
$DNCT_{i,m}$ = auxiliary variable for the linearization of bilinear terms
$DNWS_{i,s,j,m}$ = auxiliary variable for the linearization of bilinear terms
$DNZ_{i,s,s',sl,m}$ = auxiliary variable for the linearization of bilinear terms
$F_{j,p}$ = auxiliary variable for piecewise linear approximation
G_j = auxiliary variable for concision
$N_{i,j}$ = net lead time of chemical j to downstream process i
$\bar{N}_{j,l}$ = net lead time of chemical j to external market l
NS_i = number of schemes selected in process i
$NY_{i,s}$ = number of slots assigned to scheme s in process i
O_j = auxiliary variable for concision
$PD_{i,s}$ = order processing delay of scheme s
$PU_{j,k}$ = amount of chemical j purchased from external supplier k
RC_j = variance-to-mean ratio for all inputs of chemical j
$RP_{i,s}$ = variance-to-mean ratio for all inputs of scheme s in process i
$SA_{j,l}$ = amount of chemical j sold to external market l
$SC_{i,j}$ = GST of chemical j to downstream process i
$SO_{j,l}$ = GST of chemical j to external market l
$SP_{i,s,j}$ = GST of scheme s in process i to downstream chemical j
TC_j = worst case replenishment lead time of chemical j
$TP_{i,s}$ = worst case replenishment lead time of scheme s in process i
$V_{i,s,j}$ = variance of internal demand for chemical j of scheme s in process i
$W_{i,s,j}$ = amount of chemical j produced/consumed by scheme s in process i

$W^S_{i,s,j}$ = amount of chemical j produced/consumed by scheme s in process i in one cycle
$Z_{i,s,s',sl}$ = 1 if scheme s in slot sl is preceded by s' in process i
$\Gamma_{i,s,sl}$ = production time of scheme s in slot sl in process i

Literature Cited

1. Grossmann I. Enterprise-wide optimization: a new frontier in process systems engineering. *AIChE J*. 2005;51(7):1846–1857.
2. Varma VA, Reklaitis GV, Blau GE, Pekny JF. Enterprise-wide modeling & optimization—an overview of emerging research challenges and opportunities. *Comput Chem Eng*. 2007;31(5–6):692–711.
3. Wassick JM. Enterprise-wide optimization in an integrated chemical complex. *Comput Chem Eng*. 2009;33(12):1950–1963.
4. Maravelias CT, Sung C. Integration of production planning and scheduling: overview, challenges and opportunities. *Comput Chem Eng*. 2009;33(12):1919–1930.
5. Norton LC, Grossmann IE. Strategic-planning model for complete process flexibility. *Ind Eng Chem Res*. 1994;33(1):69–76.
6. Sahinidis NV, Grossmann IE, Fornari RE, Chathrathi M. Optimization model for long-range planning in the chemical industry. *Comput Chem Eng*. 1989;13(9):1049–1063.
7. Kopanos GM, Puigjaner L, Maravelias CT. Production planning and scheduling of parallel continuous processes with product families. *Ind Eng Chem Res*. 2011;50(3):1369–1378.
8. Pinto JM, Grossmann IE. Optimal cyclic scheduling of multistage continuous multiproduct plants. *Comput Chem Eng*. 1994;18(9):797–816.
9. Sahinidis NV, Grossmann IE. MINLP model for cyclic multiproduct scheduling on continuous parallel lines. *Comput Chem Eng*. 1991;15(2):85–103.
10. Sahinidis NV, Grossmann IE. Multiperiod investment model for processing networks with dedicated and flexible plants. *Ind Eng Chem Res*. 1991;30(6):1165–1171.
11. Erdirik-Dogan M, Grossmann IE. A decomposition method for the simultaneous planning and scheduling of single-stage continuous multiproduct plants. *Ind Eng Chem Res*. 2006;45(1):299–315.
12. Ierapetritou MG, Pistikopoulos EN, Floudas CA. Operational planning under uncertainty. *Comput Chem Eng*. 1996;20(12):1499–1516.
13. Liu ML, Sahinidis NV. Optimization in process planning under uncertainty. *Ind Eng Chem Res*. 1996;35(11):4154–4165.
14. Pistikopoulos EN. Uncertainty in process design and operations. *Comput Chem Eng*. 1995;19:S553–S563.
15. Zipkin PH. *Foundations of Inventory Management*. Boston, MA: McGraw-Hill, 2000.
16. Silver EA, Pyke DF, Peterson R. *Inventory Management and Production Planning and Scheduling*, 3rd ed. New York: Wiley, 1998.
17. You FQ, Grossmann IE. Stochastic inventory management for tactical process planning under uncertainties: MINLP models and algorithms. *AIChE J*. 2011;57(5):1250–1277.
18. Jung JY, Blau G, Pekny JF, Reklaitis GV, Eversdyk D. Integrated safety stock management for multi-stage supply chains under production capacity constraints. *Comput Chem Eng*. 2008;32(11):2570–2581.
19. You FQ, Grossmann IE. Design of responsive supply chains under demand uncertainty. *Comput Chem Eng*. 2008;32(12):3090–3111.
20. Erdirik-Dogan M, Grossmann IE. Slot-based formulation for the short-term scheduling of multistage, multiproduct batch plants with sequence-dependent changeovers. *Ind Eng Chem Res*. 2008;47(4):1159–1183.
21. Graves SC, Willems SP. *Supply chain design: safety stock placement and supply chain configuration*. In: Graves SC, Kok AGd, editors. *Handbooks in Operations Research and Management Science*. New York: Elsevier, 2003;11:95–132.
22. Graves SC, Willems SP. Optimizing the supply chain configuration for new products. *Manage Sci*. 2005;51(8):1165–1180.
23. Graves SC, Willems SP. Optimizing strategic safety stock placement in supply chains. *Manuf Serv Oper Manage*. 2000;2(1):68–83.
24. Inderfurth K. Safety stock optimization in multi-stage inventory systems. *Int J Prod Econ*. 1991;24(1–2):103–113.
25. Verderame PM, Elia JA, Li J, Floudas CA. Planning and scheduling under uncertainty: a review across multiple sectors. *Ind Eng Chem Res*. 2010;49(9):3993–4017.
26. Bodington EC. *Planning, Scheduling, and Control Integration in the Process Industries*. New York: McGraw-Hill, 1995.
27. Birge J, Louveaux F. *Introduction to Stochastic Programming*, 2nd ed. New York: Springer, 2011.
28. Ahmed S, Sahinidis NV. Robust process planning under uncertainty. *Ind Eng Chem Res*. 1998;37(5):1883–1892.
29. Levis AA, Papageorgiou LG. A Hierarchical solution approach for multi-site capacity planning under uncertainty in the pharmaceutical industry. *Comput Chem Eng*. 2004;28(5):707–725.
30. Papageorgiou LG, Rotstein GE, Shah N. Strategic supply chain optimization for the pharmaceutical industries. *Ind Eng Chem Res*. 2001;40(1):275–286.
31. You FQ, Grossmann IE. Mixed-integer nonlinear programming models and algorithms for large-scale supply chain design with stochastic inventory management. *Ind Eng Chem Res*. 2008;47(20):7802–7817.
32. Li J, Verderame PM, Floudas CA. Operational planning of large-scale continuous processes: deterministic planning model and robust optimization for demand amount and due date uncertainty. *Ind Eng Chem Res*. 2012;51(11):4347–4362.
33. Simpson KF. In-process inventories. *Oper Res*. 1958;6(6):863–873.
34. Clark AJ, Scarf H. Optimal policies for a multi-echelon inventory problem. *Manage Sci*. 1960;6(4):475–490.
35. You FQ, Pinto JM, Grossmann IE, Megan L. Optimal distribution-inventory planning of industrial gases. II. MINLP models and algorithms for stochastic cases. *Ind Eng Chem Res*. 2011;50(5):2928–2945.
36. You FQ, Grossmann IE. Integrated multi-echelon supply chain design with inventories under uncertainty: MINLP models, computational strategies. *AIChE J*. 2010;56(2):419–440.
37. You FQ, Grossmann IE. Balancing responsiveness and economics in process supply chain design with multi-echelon stochastic inventory. *AIChE J*. 2011;57(1):178–192.
38. You FQ, Grossmann IE, Wassick JM. Multisite capacity, production, and distribution planning with reactor modifications: MILP model, bilevel decomposition algorithm versus lagrangean decomposition scheme. *Ind Eng Chem Res*. 2011;50(9):4831–4849.
39. Humair S, Willems SP. Optimizing strategic safety stock placement in supply chains with clusters of commonality. *Oper Res*. 2006;54(4):725–742.
40. Klosterhalfen S, Minner S. *Comparison of stochastic- and guaranteed-service approaches to safety stock optimization in supply chains*. In: Waldmann K-H, Stocker UM, editors. *Operations Research Proceedings 2006*, *Vol*. 2006. Berlin/Heidelberg: Springer, 2007:485–490.
41. Wolsey LA. MIP modelling of changeovers in production planning and scheduling problems. *Eur J Oper Res*. 1997;99(1):154–165.
42. Tawarmalani M, Sahinidis NV. A polyhedral branch-and-cut approach to global optimization. *Math Program*. 2005;103(2):225–249.
43. Kondili E, Pantelides CC, Sargent RWH. A General algorithm for short-term scheduling of batch operations. 1. MILP formulation. *Comput Chem Eng*. 1993;17(2):211–227.
44. Rosenthal RE. *GAMS—A User's Guide*. Washington, DC: GAMS Development Corporation, 2011.
45. Glover F. Improved linear integer programming formulations of nonlinear integer problems. *Manage Sci*. 1975;22(4):455–460.
46. Nemhauser GL, Wolsey LA. *Integer and Combinatorial Optimization*. New York: Wiley, 1999.
47. Padberg M. Approximating separable nonlinear functions via mixed zero-one programs. *Oper Res Lett*. 2000;27(1):1–5.
48. Croxton KL, Gendron B, Magnanti TL. A comparison of mixed-integer programming models for nonconvex piecewise linear cost minimization problems. *Manage Sci*. 2003;49(9):1268–1273.

Appendix

Theorem 1. *Constraints 5–8, in conjunction with the integrality of the assignment variables $SY_{i,s,sl}$ lead to the following unique solution*

$$Z_{i,s,s',sl} = SY_{i,s',sl-1} \cdot SY_{i,s,sl} \tag{A1}$$

where the transition variables $Z_{i,s,s',k}$ are treated as nonnegative continuous variables.

Proof: Consider an arbitary flexible process l, two arbitrary production schemes m and n, and an arbitrary time slot

k. Assume $SY_{l,m,k-1} = 1$ and $SY_{l,n,k} = 1$. From (5), we know that for each flexible process $i \in FL$, exactly one scheme can be assgined to slot sl, and exactly one scheme can be assigned to slot $sl - 1$. Therefore

$$SY_{l,s,k-1} = 0, \quad \forall s \neq m \tag{A2}$$

$$SY_{l,s,k} = 0, \quad \forall s \neq n \tag{A3}$$

From (A2), (A3), and (6)–(8) we know that

$$Z_{l,s,s',k} = 0, \quad \forall s, \forall s' \neq m \tag{A4}$$

$$Z_{l,s,s',k} = 0, \quad \forall s', \forall s \neq n \tag{A5}$$

Now (A4) and (A5) indicate that $Z_{l,s,s',k}$ can be nonzero only for $s' = m$ and $s = n$. Furthermore, according to (6) and (7), at least one $Z_{l,s,s',k}$ must be one. Therefore

$$Z_{l,s,s',k} = SY_{l,s',k-1} \cdot SY_{l,s,k} = 0, \quad \forall s \neq n, s' \neq m \tag{A6}$$

$$Z_{l,m,n,k} = SY_{l,m,k-1} \cdot SY_{l,n,k} = 1 \tag{A7}$$

Hence, although $Z_{l,s,s',k}$ are relaxed as continuous variables in interval [0, 1], they can only take the values of either 0 or 1. ■

Manuscript received Jun. 30, 2012, and revision received Sept. 6, 2012.