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Managing Risk through a Flexible Recipe Framework

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A novel approach is proposed that exploits the use of a flexible recipe framework as a better way to handle the risk associated with the scheduling under uncertainty of batch chemical plants. The proposed solution strategy relies on a novel two-stage stochastic formulation that explicitly includes the trade-off between risk and profit at the decision-making level. The model uses a continuous-time domain representation and the generalized notion of precedence. Management of risk is explicitly addressed by including a control measure (i.e., the profit in the worst scenario), as an additional objective to be considered, thus, leading to a multiobjective optimization problem. To overcome the numerical difficulties associated with such mathematical formulation, a decomposition strategy based on the sample average approximation (SAA) is introduced. The main advantages of this approach are illustrated through a case study, in which a set of solutions appealing to decision makers with different attitudes toward risk are obtained. The potential benefits of the proposed flexible recipe framework as a way of managing the risk associated with the plant operation under demand uncertainty are highlighted through comparison with the conventional approach that considers nominal operating conditions. Numerical results corroborate the advantages of exploiting the capabilities of the proposed flexible recipe framework for risk management purposes. *AIChE J,* 54: 728–740, 2008
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Introduction

During the past decades the chemical industry has been faced with a major change in which companies are required to operate within a competitive and changing market and meet stricter product specifications. In this context, process operations optimization can effectively increase plant profitability while ensuring at the same time that safety and profit quality requirements are also met.[1–3] Furthermore, special interest is focused on the production of high-value added and high-technology chemicals whose processing requires complex synthesis and separation steps. The inherent flexibility of batch processes makes this mode of operation very attractive for such scenario.

Scheduling is a very important issue in process operations that deals with the allocation of a set of limited resources over time to manufacture a number of products, so as to optimize the short term plant productivity. The scheduling

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problem in the chemical industry has been extensively studied, and alternative methodologies and problem statements with different considerations have been proposed in the literature to address the combinatorial character of these problems.[4] With the recent trend of building smaller and flexible plants that follow the market dynamics closer, there has been a renewed interest in batch processes.[5] As a result of this, a high-effort is being devoted to the development of different strategies and tools for modeling, simulation and optimization of these processes.[6] Thus, the area of process scheduling has been the focus of a growing research interest in recent years. Extensive reviews can be found in the literature.[7–10]

In batch processing, a production recipe is traditionally defined as the entity containing all the information concerning the sequence of tasks to be performed so as to make a given product. Most of the scheduling approaches assume that batch processes are operated at nominal conditions following predefined fixed production recipes. However, such ideal conditions are very rare in practice and chemical plants often operate under conditions quite different from those considered at the design stage. This traditional way of operation, called in this work fixed recipe operation, does not permit adjustments in plant resources availability variations either in the quality of raw materials or in the actual process conditions. On the other hand, a flexible recipe operation is a suitable way of incorporating systematic recipe adaptations depending on the actual process conditions.

Recipe flexibility

The flexible recipe concept was originally introduced as a set of adaptable recipe items that controls the process output, and can be modified to face any deviation from the nominal conditions.[11] Technically, the nominal recipe for a given product represents the optimal compromise between quality and costs for a given batch regardless of the production environment where this batch will be produced. However, recipes should be changed or modified to some extent according to the specific features of the production scenario. For instance, in case of a catalytic process, deviations in the feed quality could be compensated by means of an increase in the amount of catalyst in order to obtain a constant output. Alternatively, in some reactions, an increase of the heating rate might be useful when the production needs to be accelerated by shortening the reaction times. A simple example can be found in the bakery industry, where the temperature of the ovens can be tracked with the intention of controlling the residence time of the bread inside. For this reason, recipes are adapted in practice, but usually in a rather unsystematic way that relies on the experience and intuition of the operators. Verwater-Lukszo developed this basic idea and introduced the concept of flexible recipe as a way of systematically adjusting the control recipes during the execution of the production tasks.[12] This methodology was applied to several experiments where small modifications in the nominal conditions were considered. The aim was to observe the process performance under different operating conditions. Since then, several authors have applied the same approach to optimize other chemical processes.[13,14] Specifically, Romero et al. developed one of the first attempts to extent the flexible recipe approach to a plant-wide scheduling problem.[15] This work proposed to optimize the production scheduling of a batch plant where the recipes had some kind of flexibility. These authors integrated a linear flexible recipe model into a multipurpose batch process scheduling formulation based on graph theory. In their work, the flexible recipe model allowed the integration between a recipe optimization procedure at the control level and a batch plant optimization strategy.

Scheduling under uncertainty

In addition to the control problem, the complexity of the scheduling problem is further increased by the high-degree of uncertainty brought about by external factors, such as continuously changing market conditions and customer expectations, and internal parameters, such as product yields, qualities and processing times. Although the research community has repeatedly recognized the importance of incorporating uncertainties in the scheduling formulations, most of the models developed so far in the literature are deterministic. Such models, assume that all the problem data are known in advance, and provide solutions whose accuracy depend on the degree of uncertainty.

Specifically, a literature survey reveals that the most important and extensively studied source of uncertainty has been demand.[16–20] The emphasis on incorporating demand uncertainty into the planning decisions is appropriate given the fact that meeting effectively customer demand is what mainly drives most planning initiatives.

The scheduling of batch plants under demand uncertainty has recently emerged as an important research area. Some attempts in scheduling under uncertainty have focused on rescheduling algorithms. These approaches are reactive strategies that are implemented when the uncertainty is actually unveiled. Here, the scheduling decisions are calculated depending on the actual state of the plant, and without considering the future possible outcomes of the uncertain parameters.[21] On the other hand, proactive approaches are those in which the uncertainty associated with the model data is considered *a priori*. The goal is to calculate a robust schedule able to cope with the possible outcomes of the uncertain parameters. Specifically, the prevalent proactive approach in scheduling under uncertainty has been multistage stochastic programming. This strategy deals with problems involving a sequence of decisions that react to outcomes that evolve over time. In this type of models, at each stage, one makes decisions based on currently available information, i.e., past observations and decisions, prior to the realization of the uncertain future events.

Stochastic approaches differ primarily in the selection of the decision variables and the way in which the expected value term, which involves a multidimensional integral accounting for the probability distribution of the uncertain parameters, is calculated. Specifically, two distinct methodologies for representing uncertainty can be identified within probabilistic methods. These are the scenario-based approach and the distribution-based approach.

In the first approach,[22–26] the uncertainty is described by a set of discrete scenarios capturing how the uncertainty might play out in the future. Each scenario is associated with a probability level representing the decision maker's expectation of the occurrence of a particular scenario. The scenario-based approach avoids the problem of multivariate integration when the random variables follow multidimensional continuous distributions. This is achieved by generating a finite set of scenarios, from sampling of a discrete approximation of the given distributions, to represent the probability space. With the scenarios or scenario tree specified, the stochastic program becomes a deterministic equivalent program.

In cases where a natural set of discrete scenarios cannot be identified, and only a continuous range of potential futures can be predicted, the distribution-based approach is used. By assigning a probability distribution to the continuous range of potential outcomes, the need to forecast exact scenarios is obviated. The distribution-based approach is adopted by some research works, in which demand is modeled as normally distributed with a specified mean and standard deviation.[27,16,17]

One of the key issues that has not been properly addressed in the literature is that of managing the risk associated with the scheduling problem under uncertainty. Although stochastic models optimize the total expected performance measure, they usually do not provide any control on its variability over the different scenarios, i.e., they assume that the decision-maker is risk neutral. However, different attitudes toward risk may be encountered. In general, most decision-makers are risk averse implying a major preference for lower variability for a given level of return.[28] Specifically, the extension of the objective beyond simple expectations was presented by Ahmed and Sahinidis, who argued that robustness should also be sought.[4] They penalized downside risk, defined in their work as costs above the expected cost. Applequist et al. also recognized that simply optimizing expected returns can lead to higher risk solutions.[29] Bonfill et al. presented some techniques to manage financial risk in scheduling problems,[30] similarly to the way it was done by Barbaro and Bagajewicz for planning problems.[28] Some of these techniques have also been used for manipulating the financial risk in the area of scheduling and design of supply chains under demand uncertainty.[31,32]

Scope of the work

This work provides a tool to support the scheduling under uncertainty of batch chemical processes taking full advantage of the flexible recipe framework. Specifically, the aim of the model is to balance the trade-off between a high-demand satisfaction level, which can be achieved by keeping high-inventories, and low-inventory costs, which may imply leaving part of the demand unsatisfied. In this context, the flexible recipe framework is used to increase the production rate, and, thus, the final inventories. This is done through variations in the parameters of the flexible stages of the recipe.

To address this problem, a large-scale multiobjective stochastic mixed-integer-linear-programming (MILP) model is presented. This model is based on the general precedence model,[33,34] and explicitly includes the trade-off between risk and profit. The outcome of such formulation consists of a set of Pareto-optimal solutions from which the decision-maker should choose the best one according to his/her preferences. To our knowledge, this is the first approach that exploits the concept of flexible recipe within a risk management framework. In the resulting strategy, the detailed decisions associated with the control recipe are calculated in conjunction with those dealing with the scheduling tasks. This integrated way of operation increases the batch plant flexibility and its capability of giving a quick response to the market trends.

This article is organized as follows: The problem definition is outlined first, along with the assumptions considered. Then, the proposed stochastic formulation accounting for the maximization of the expected profit is given. The inclusion of an explicit control measure to manage risk is addressed in the following section. The effectiveness of the proposed approach as a decision-making tool is next illustrated through its application to a scheduling case study. Finally, some concluding remarks are given at the end of the work.

Problem statement

Given are several products that are to be manufactured on a multistage multipurpose batch plant within a scheduling time horizon. Thus, the following data is assumed to be known in advance:

- Set of raw materials, intermediate and final products to be manufactured.
- Set of production recipes, fixed batch sizes and prices of final products.
- Topology of the plant, i.e., number of equipment units, their capacities and suitabilities for the labor tasks.
- Cost functions associated with raw materials and utilities consumption, holding inventory over the horizon and penalties for unsatisfied demand.

Sales of products are assumed to be executed at the end of the time horizon. The demand associated with each product cannot be perfectly forecasted, and its uncertainty is represented by a set of scenarios with given probability of occurrence. Decisions regarding scheduling tasks are made prior to the realization of the uncertain parameter. Therefore, while the scheduling decisions (number of tasks to be performed, batch sizes, assignment and sequencing decisions) must be taken at the beginning of the time horizon, that is, prior to the demand realization, sales are computed once the random events take place at the end of it. Thus, the problem contemplated involves two types of decisions. The first stage ones, i.e., scheduling decisions and purchases of raw materials, must be calculated bearing in mind the demand uncertainty. The second stage ones, i.e., sales of final products, are taken in order to react to the outcome of the uncertain parameter, i.e., demand realization. Then, the stochastic problem consists of finding the scheduling decisions that maximize the total expected profit, which is computed over a set of demand scenarios. This profit term is calculated from the sales revenues, operating costs, inventory costs and unsatisfied demand costs. This overall two-stage stochastic framework strategy is illustrated in Figure 1.

Mathematical formulation

The indices, parameters, and variables included in the model are defined in the notation section. The MILP formulation is next described in detail.

Flexible Recipe Model. Our formulation is based on a flexible recipe model that relates deviations of process outputs to the deviation of the main flexible recipe items. Deviations of the recipe item f of a task involved in the manufac-

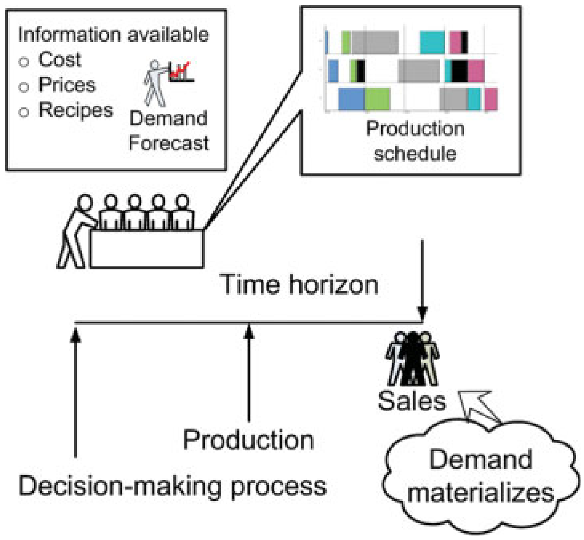

Figure 1. Two-stage stochastic framework.

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

turing stage s of batch i belonging to product p from its nominal value is denoted by the continuous variable $\delta_{pisf.}$ This flexible recipe model can be either expressed in an explicit or implicit form. In the explicit form the output deviations are expressed as a function of the input recipe items. On the other hand, in the implicit form, which is used in constraint (Eq. 1), all the terms of the equation are placed on the lefthand side of the equality. Note that in this latter case the output parameters of the flexible model have negative signs, whereas the input ones are positive ($lfmod_{psf}$).Thus, looking at the plant as a whole, a flexible recipe model enables varying the processing times of the tasks by tracking other recipe parameters (i.e., amount of catalyst, temperature, etc.) so as to optimize the global performance of the process. In this context, the end-point condition of any stage is a recipe input of the following one. Furthermore, the process output deviations can be set to zero, or constrained to take values within a specific interval according to the features of the case study being analyzed. In this work, a linear flexible recipe model has been adopted, but the model could easily be adapted to more complex situations

$$\sum_{f\in FP_{ps}} lfmod_{psf}\delta_{pisf}=0 \quad \forall p\in P,\ i\in I_P,\ s\in S_P,\ (p,s)\in FL_{ps} \quad (1)$$

Notice, that in some cases the aforementioned linear model may be a linear approximation of a nonlinear model, and will only be valid within a specific operating range. Thus, these constraints establish the maximum negative ($fplb_{psf}$) and positive deviations ($fpub_{psf}$) allowed for each recipe item

$$fplb_{psf} \le \delta_{pisf} \le fpub_{psf} \quad \forall p\in P,\ i\in I_P,\ s\in S_P,\ (p,s)\in FL_{ps},\ f\in FP_{ps} \quad (2)$$

Allocation constraints

We define a binary variable denoted by Y_{pisu} that takes the value of 1 if batch i belonging to product p is manufactured, and its s^{th} stage is allocated to unit u and 0, otherwise. The following constraint (Eq. 3) enforces the assignment of a single processing unit to a task (p, i, s) if this batch is produced

$$\sum_{u\in U_{ps}} Y_{pisu} \le 1 \quad \forall p\in P,\ i\in I_P,\ s\in S_P \quad (3)$$

Equation 4 forces the condition for which the nonproduced batches are located at the end of the schedule, i.e., it ensures that the decision to manufacture a batch of a product is only taken if its preceding batch is also produced. Although this constraint is not needed formally, it helps computations. Indeed, by fixing the position of the nonproduced batches we get smaller branch-and-bound trees and shorter computational times. The specific position of these nonproduced batches (at the end of the schedule) is absolutely arbitrary, and is chosen for simplicity

$$\sum_{u\in U_{ps}} Y_{pisu} \ge \sum_{u'\in U_{ps'}} Y_{pi's'u'} \quad \forall p\in P,\ i,i'\in I_P,\ s,s'\in S_P : i'>i \quad (4)$$

Scheduling horizon constraints

Constraint 5 states that every production task involved in the manufacturing stage s of batch i belonging to product p must be completed within the specified scheduling horizon of length H

$$FT_{pis} \le H \quad \forall p\in P,\ i\in I_P,\ s\in S_P \quad (5)$$

Timing constraints

The following constraints establish the duration of a task considering the processing times of the recipes. Thus, Eq. 6 states that a task cannot finish before its starting time, plus the nominal processing time and the deviations of the processing time. Let us note that these deviations are only allowed in the flexible recipe stages

$$FT_{pis} \ge ST_{pis} + npt_{ps} + \delta_{pisDTOP} + tt_{ps} \quad \forall p\in P,\ i\in I_P,\ s\in S_P \quad (6)$$

Sequencing constraints

$X_{pisp'i's'}$ is a sequencing binary variable which establishes a relation of general precedence between two different tasks of the same type (p, i, s) and (p', i', s') executed in the same processing unit.

Constraint 7 is added to ensure that task (p', i', s') is not started before the completion of task (p, i, s) if the former task (p, i, s) precedes the latter task (p', i', s'), and both are executed in the same unit. Constraints 8 is equivalent to constraint 7, but is applicable for the opposite case, that is, when task (p', i', s') precedes task (p, i, s)

$$ST_{p'i's'} \ge FT_{pis} - M(1-X_{pisp'i's'}) - M(2-Y_{pisu}-Y_{p'i's'us})$$
$$\forall p,p'\in P,\ i,i'\in I_P,\ s,s'\in S_P,$$
$$u\in (U_{ps}\cap U_{p's'}) : (p<p')\cup(p=p',s<s') \quad (7)$$

$$ST_{pis} \ge FT_{p'i's'} - M(1-X_{pisp'i's'}) - M(2-Y_{pisu}-Y_{p'i's'u})$$
$$\forall p,p'\in P,\ i,i'\in I_P,\ s,s'\in S_P,$$
$$u\in (U_{ps}\cap U_{p's'}) : (p<p')\cup(p=p',s<s') \quad (8)$$

Constraint 9 sequences pairs of batches of the same product, provided that both batches are manufactured

$$ST_{pi's} \geq FT_{pis} - M(1 - Y_{pi'su}) \quad \forall p \in P,\ i, i' \in I_P,\ s \in S_P,\ u \in U_{ps} : i < i' \quad (9)$$

Constraint 10 is defined for every pair of consecutive processing stages that must be sequentially performed for a particular product. This constraint is applied in conjunction with constraint 6 in order to describe a nonintermediate storage policy (NIS). Within a NIS policy, there is not any intermediate storage tank available between consecutive tasks. Then, an equipment unit is not free until it finishes processing, and the intermediate product is transferred to the equipment unit assigned to the next task. In this type of general precedence models, different storage policies may be easily adopted by changing the signs of the corresponding inequalities[34]

$$FT_{pis} - tt_{ps} = ST_{pis'} \quad \forall p \in P,\ i \in I_P,\ s, s' \in S_P : s' = s + 1 \quad (10)$$

Demand constraints

Equation 11 states that the sales can be lower or equal to the demand as our model assumes that some of the demand can be left unsatisfied because of limited production capacity

$$SALES_{pe} \leq dem_{pe} \quad \forall p \in P,\ e \in E \quad (11)$$

Moreover, Eq. 12 constraints the sales to be lower or equal to the amount produced, plus the available inventory from the previous period, which is computed through Eq. 13

$$SALES_{pe} \leq QP_p + IN_p^{ini} \quad \forall p \in P,\ e \in E \quad (12)$$

where the amount produced QP_p is computed is computed through Eq. 13

$$QP_p = \sum_{i \in I_P} \sum_{s = \{s_p^l\}} \sum_{u \in U_{ps}} bsz_p Y_{pisu} \quad \forall p \in P \quad (13)$$

Here, the amount of each product manufactured in the plant is calculated from the batch sizes of the products, and the binary variables representing the existence of these batches.

Inventory constraints

These constraints are added to calculate the average inventory of each product (Eq. 14) from the batch size and the finishing time of each batch of product p

$$IN_p = \sum_{i \in I_P} \sum_{s = \{s_p^l\}} bsz_p \frac{(H - FT_{pis})}{H} \quad \forall p \in P \quad (14)$$

Objective function

This model accounts for the maximization of the total expected profit (Eq. 15), which is computed by calculating the average of profits over the entire range of scenarios. The profit values in each scenario are computed through Eq. 16. This equation assumes that revenues are obtained through sales of final products, while costs are due to holding inventories, consumption of utilities and raw materials, and the underproduction, i.e., leaving part of the demand unsatisfied. An additional term accounting the cost associated to the deviation of the recipe from its nominal parameters has been also considered in this expression

$$\max \quad E[PFS] = \sum_{e \in E} prob_e \cdot PFS_e \quad (15)$$

$$PFS_e = \sum_{p \in P} \Big(SALES_{pe} sp_p - IN_p Hpinv_p - QP_p pc_p - udc_p (dem_{pe} - SALES_{pe}) \Big) - \sum_{p \in P} \sum_{i \in I_p} \sum_{s \in S_p} \sum_{f \in FP_{ps}} dcost_{psf} \delta_{pisf} \quad \forall e \in E \quad (16)$$

The overall stochastic model without risk management considerations can be expressed as follows (so-STOC)

$$\max \quad E[PFS]$$

subject to

constraints 1-16

Risk management

The proposed stochastic optimization MILP model attempts to account for uncertainty by optimizing the expected profit without reflecting and controlling the variability of performances associated with each specific scenario. Although the schedules obtained could be considered more robust than the deterministic ones, based on nominal parameter values, by taking a purely expected profit maximization perspective, the model assumes that the decision maker is risk-neutral or indifferent to profit variability. Therefore, there is no guarantee that the process will perform better at a certain level considering the whole uncertain parameters space. The only guarantee is that the average is optimized.[35,36]

The idea underlying risk management is the incorporation of the trade-off between risk and profit within the decision-making process. This leads to a multiobjective optimization problem in which the expected performance and a specific risk measure are the objectives considered. In our work, the probability of meeting unfavorable scenarios is controlled by adding the worst-case profit as an additional objective to be maximized. A major difference with respect to other probabilistic metrics, such as the financial risk[28] or the downside risk[37] is that the probability information of the problem cannot be explicitly used when manipulating the worst case. Nevertheless, this metric has been shown to be very effective in identifying robust schedules. Furthermore, it is easy to implement, and leads to a good numerical performance in two-stage stochastic models.[30]

These both issues have motivated its application to our specific problem

$$WC \leq PFS_e \quad \forall e \in E \quad (17)$$

The worst case profit can be computed through Eq. 17, and the inclusion of this term as an alternative objective to be maximized along with the expected profit leads to the following multiobjective formulation (mo-STOC)

$$\begin{aligned} &\max \quad \{E[PFS], WC\} \\ &\text{subject to} \\ &\quad \text{constraints 1-17} \end{aligned} \tag{18}$$

The aforementioned multiobjective problem can be solved by standard algorithms for multiobjective optimization,[38] such as aggregation methods, the ε-constraint or the goal programming algorithms. Moreover, the problem can be reformulated as a multiparametric mixed integer programming problem,[39] which can then be solved using recently developed algorithms for parametric optimization.[40] Specifically, our work applies an enumeration-based approach based on the ε-constraint method,[41] to generate the efficient solutions for the multiobjective problem that accounts for the maximization of the expected profit and the worst case profit. The multiparametric problem that has to be solved can be expressed as follows (p-STOC)

$$\begin{aligned} &\max \quad E[PFS] \\ &\text{subject to} \\ &\quad \text{constraints 1-17} \\ &\quad WC \geq \theta \\ &\quad \theta \in \left[\theta^L, \theta^U\right] \end{aligned} \tag{19}$$

where θ^L is given by the value of the worst case profit in the maximum expected profit solution, that is

$$\theta^L = \max[PFS_e] \tag{20}$$

Here, PFS_e represents the profit value attained by the maximum expected profit solution in each scenario. Let us note that this solution is obtained by maximizing the expected profit, and without considering any financial risk control measure. On the other hand, the value of θ^U is the optimal solution of the following single-objective problem

$$\begin{aligned} &\max \quad WC \\ &\text{subject to} \\ &\quad \text{constraints 1-17} \end{aligned} \tag{21}$$

Thus, after computing the lower and upper bounds of θ the resulting interval is discretized into NQ sufficiently small subintervals, and the ε-constraint method is then applied at each parameter interval realization.[38] In our case, NQ single optimization problems as the one presented earlier (Eq. 19), should be computed. The specific values of θ are calculated from Eq. 22

$$\theta^1 = \theta^L; \qquad \theta^q = \theta^L + \frac{\theta^U - \theta^L}{NQ}; \qquad \theta^{NQ} = \theta^U; \tag{22}$$

Once all the NQ solutions have been computed, an additional post-processing step is required for detecting efficiency, based on the concept of dominance.[41] A solution A is said to be dominated by another solution B, if the expected profit and worst case values associated with solution B, are both greater or equal to those associated with solution A, and at least one of them is strictly greater. Thus, this last step of the algorithm has to be included as part of the overall multiobjective optimization algorithm, and focuses on discarding those solutions which are dominated by at least one of the others. A solution is considered to be Pareto-optimal if it is not dominated by any other solution.

Decomposition Technique

The approach presented previously, leads to a large-scale mo-MILP. This model may become computationally expensive in real industrial scenarios with complex plant topologies and high-number of different products and process recipes. The complexity of this formulation may be further increased by the high-number of scenarios required to capture the demand uncertainty.

Thus, in this section a decomposition strategy is introduced aiming at the objective of overcoming the numerical difficulties associated with the approach described in the previous section. The proposed strategy is based on the sample average approximation[42] (SAA). The underlying idea consists of using a variation of this technique to approximate the solution of the mo-MILP that accounts for the maximization of the expected profit and worst case. Here, the SAA is used as a way of generating a set of candidate solutions that exhibit different risk performances, and whose Pareto optimality, in terms of expected profit and worst case, must be checked, based on the concept of dominance. The proposed method to manage risk has similar features to the one suggested by Aseeri et al.[43]

In general terms, the SAA is an approach for solving single objective stochastic optimization problems by using Monte Carlo simulation.[42] In the SAA technique, the expected second-stage profit (recourse function) in the objective function is approximated by an average estimate of NS independent random samples of the uncertain parameters, and the resulting problem is called approximation problem. Here, each sample corresponds to a possible scenario. Then, the resulting approximation problem is solved repeatedly for R different independent samples (each of size NS) as a stochastic optimization problem of size NS. The average of the objective function of the approximation problems provides an estimate of the stochastic problem objective. Notice that this procedure may generate up to R different candidate solutions. To determine which of these R (or possibly less) candidates is optimal in the original problem, the values of the first-stage variables corresponding to each candidate solution are fixed and the problem is solved again using a larger number of scenarios $NS' \gg NS$ in order to distinguish the candidates better. After solving these new problems, the optimal solution of the original problem $(\hat{x}^e)$ is determined. Therefore, $\hat{x}^e$ is given by the solution of the approximate problems that yields the highest objective value for the approximation problem with NS' samples.

In this article, we apply a variation of the SAA that aims to calculate the set of efficient solutions to the multiobjective formulation that simultaneously accounts for the maximization of expected profit and worst case (i.e., mo-STOC). In our approach, the problem is solved deterministically for each scenario, in other words, $NS = 1$; $R = |E|$ and $NS' = |E|$. This provides a set of first-stage decision variables (i.e., schedules) that must be evaluated in the uncertain parameters

Table 1. Recipe Parameters and Flexibility Region Around the Nominal Conditions for the Cross-Cannizaro Reaction Recipe Model

Flexible recipe item	Deviation variable	Flexibility Region fplp	Flexibility Region fpub	dcost
δ_{DPS}	yield	0*	0*	–*
δ_{DTEMP}	temperature	−0.7 °C	0.5 °C	0.03 m.u./°C
δ_{DTOP}	duration	−1.25 h	0.5 h	0.02 m.u./h
δ_{DKOH}	amount of KOH	−27 g	8.5 g	0.05 m.u./kg
δ_{DFOR}	amount of Formaldehyde	−30 g	7.5 g	0.04 m.u./kg

*No deviation is allowed in quality.

space. Thus, the second stage decision variables (sales and inventory profiles) associated with each of these deterministic solutions are calculated by fixing the deterministic schedules in the stochastic problem and solving it. The stochastic problem is the original single-objective two-stage model with |E| scenarios that maximizes the expected profit (so-STOC). In such model, the combinatorial complexity is eliminated by fixing the scheduling decisions. This provides, for each schedule being assessed, the expected profit, and the worst case attained under the uncertain environment. Finally, the solutions are filtered in terms of expected profit and worst case by applying the dominance concept. Those solutions that are dominated in terms of the predefined criteria are discarded from the original set, whereas the set of nondominated schedules are stored. The latter ones constitute the approximated solution to the original problem. For a stochastic problem of type mo-STOC with |E| scenarios, the proposed algorithm can be summarized as follows:

begin
  for e = 1 to |E| do
    solve the deterministic problem for scenario k.
    Let $\hat{x}^e$ be the optimal solution of the problem;
    store the first stage decisions (i.e., schedules) associated with $\hat{x}^e$;
    fix the first stage decisions in the stochastic problem with |E| scenarios (so-STOC) and solve it;
    store the expected profit and worst case associated with $\hat{x}^e$;
  end for
  filter the solutions $\hat{x}^e$ by applying the dominance concept;
end

This algorithm provides an approximation (i.e., lower bound) to the original Pareto frontier of the problem. Let us note that the computational resources associated with the proposed algorithm can be decreased by reducing the optimality gap, as well as the maximum CPU time imposed to the so-MILPs to be solved.

Case Study

The advantages of our proposed framework will be illustrated by the batch-wise production of benzyl alcohol. The crossed-Cannizaro reaction for the production of benzyl alcohol has been studied by Keesman who proposed a quadratic model to predict the yield of the reaction (DPS) for *a priori* known disturbances in the process inputs (DTEMP, DTOP, DKOH and DFOR).[44] In this work, we apply a linear approximation of the aforementioned model, which was also used by Romero et al.[15] Such approximation leads to Eq. 23 presented in its explicit and implicit forms

$$\delta_{DPS} = 4.4\delta_{DTEMP} + 4\delta_{DTOP} + 95\delta_{DKOH} + 95\delta_{DFOR} \rightarrow \delta_{DPS} - 4.4\delta_{DTEMP} - 4\delta_{DTOP} - 95\delta_{DKOH} - 95\delta_{DFOR} = 0 \quad (23)$$

Table 1 shows the flexible recipe items considered for this reaction, and the valid flexibility region around the nominal operating conditions. Data for the production of benzyl alcohol are shown in Table 2. Transfer times have been considered equals to the 5% of the processing times. This case study consists of four products, P1 to P4, which must be processed over a 112-h horizon in a multistage multipurpose batch plant. Initial inventory is assumed to be inexistent at the period of time considered. It is assumed that the demand

Table 2. Problem Data

Product Stages	P1 Unit	P1 npt, h	P2 Unit	P2 npt, h	P3 Unit	P3 npt, h	P4 Unit	P4 npt, h
1	U1	2	U3	6	U4	4	U2	7
2	U2	7	U1	6	U2	8	U1	2
3	U3	8	U2	8	U3	6	U4	6
4	U4	4	U4	8	U1	4	U3	4
bsz_p, kg/batch	40		55		40		35	
mpc_p, kg	160		110		120		105	
$mdem_p$, kg	280		110		120		120	
$demdev_p$, %	30		35		40		40	
sp_p, m.u./batch	70		55		40		40	
pc_p, m.u./batch	8		7		5		8	
$pinv_p$, m.u./h	1		2		1.1		0.5	
udc_p, m.u./kg	4		3		2		3	

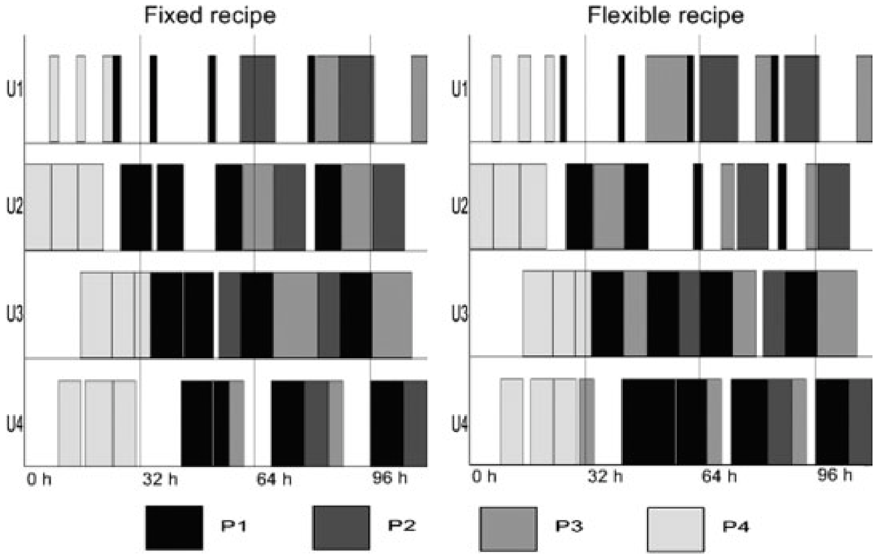

Figure 2. Gantt-charts of the stochastic solutions.

cannot be perfectly forecast, and its uncertainty is represented by 100 equiprobable and independent scenarios. These scenarios are generated by applying a Monte Carlo sampling over a set of probability functions. Specifically, the scenarios are calculated assuming that the demand of each product follows a normal probability distribution. The production rates (*bsz*), maximum plant capacity (*mpc*), selling prices (*sp*), and production costs (*pc*), are also given in Table 2, as well as the market information, namely the mean demands (*mdem*), their standar deviations (*demdev*) and the unsatisfied demand costs (*udc*).

The second stage of products P1 and P2, and the first stage of product P4, which involve the reaction required for the production of benzyl alcohol, follow the flexible recipe model previously presented in Eq. 23. Furthermore, following the work of Romero et al.[15] we have considered that the first stage of product P1 executed in unit U1 is also flexible. This is in fact a preheating stage in which end-point temperature (DTEMP) is assumed to increase linearly with time (DTOP)

$$\delta_{DTEMP} = 10\delta_{DTOP} \rightarrow \delta_{DTEMP} - 10\delta_{DTOP} = 0 \qquad (24)$$

The final temperature achieved by this task corresponds to the temperature for the reaction in the next stage. Therefore, shorter preheating times in this stage will have to be compensated in the following reaction stage Finally, no restrictions on time deviations have been assumed for this stage.

The stochastic approach that maximizes expected profit and neglects risk management is solved in the first place. The model is implemented within the modeling language GAMS, and solved with the MIP solver of CPLEX version 9.0.[45] The mathematical formulation involves 1,569 constraints, 653 continuous variables, and 224 binary variables. Specifically, two models are solved, the first one for the fixed recipe case, and the second one assuming a flexible recipe framework. The fixed recipe model leads to an expected profit of 15,348.4 m.u., while the flexible one yields 15,858.7 m.u. The schedules associated with both solutions are shown in Figure 2.

As can be observed, the improvement in the objective function value is achieved by producing one more batch of product P3. To do so, the flexible recipe framework takes advantage of its capability of reducing the processing times. This results in an extra recipe modification cost, which is compensated by the increase in the sales revenues, thus, leading to an overall better solution in terms of the proposed objective function. Furthermore, comparing both schedules, several sequencing decisions have been changed in order to accommodate this additional batch while using the flexible recipe framework.

The trade-off between risk, which is assessed by using the worst-case profit, and the expected profit, is next investigated by solving the multiobjective MILP model that accounts for the maximization of both criteria. The problem is solved in two different ways. The first one is the enumeration-based approach, based on the ε-constraint method,[41] which consists of parametrically varying the value of the lower bound imposed to the worst-case metric θ The second one is the strategy, based on the SAA algorithm. With regard to the latter, let us note that it decomposes the original two-stage stochastic problem with 100 scenarios into 100 deterministic problems that are solved for every scenario *e* in the original formulation. To increase the speed of the algorithm, we impose a limit of 100 CPU s, and an optimality gap of 5% for every deterministic subproblem. The results obtained in both cases are illustrated in Figure 3. The figure also depicts the efficient solutions associated with the fixed recipe mode of operation.

From the set of efficient solutions of the problem, it is clear that in both cases (i.e., fixed and flexible recipe modes of operation) a conflict exists between both objectives (i.e., maximum expected profit and maximum worst case). Thus, results indicate that an improvement in the worst case is only possible if the decision-maker is willing to compromise the expected profit. Certainly, schedules with better worst-case values will reduce the risk, but at the expense of a reduction in the value of the expected profit. The effectiveness of introducing flexible recipes is justified by the fact that the curve

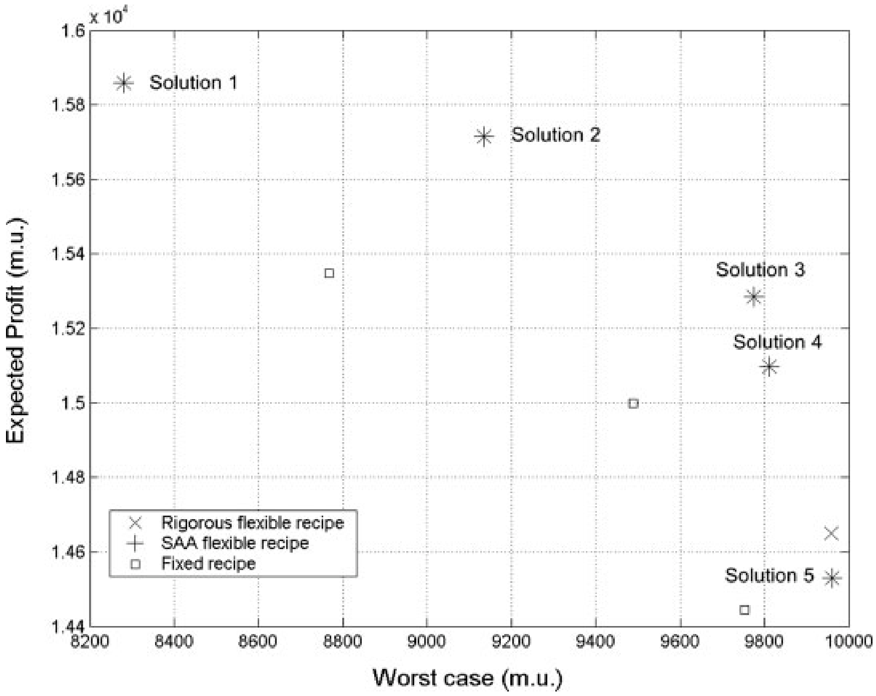

Figure 3. Optimal-pareto solutions for fixed and flexible recipe frameworks.

obtained using flexible recipe lies entirely above the one associated with the fixed recipe. This implies that for any worst-case value the flexible recipe framework always leads to a higher expected profit. Specifically, the difference between both expected profits ranges from 2 to 6% depending on the specific worst case value being analyzed. Moreover, the use of the flexible recipe allows attaining solutions with higher worst-case values, which are impossible to achieve otherwise by using fixed recipes. In fact, the maximum worst-case solution computed with the flexible recipe formulation is equal to 9,774 m.u., whereas the fixed recipe model is not able to provide solutions with a worst case higher than 9,960 m.u. This analysis provides valuable information to the decision maker and indicates that the inclusion of flexible recipes in a batch plant manufacturing environment leads to a more effective way of managing the associated risk.

With regard to the proposed decomposition strategy, let us note that it shows a good numerical performance, as it is able to detect five out of the six Pareto-optimal solutions identified by the rigorous approach. These solutions are summarized in Table 3, while Figure 4 includes their corresponding Gantt charts. By inspecting in detail these schedules, we can see how all the batches of P1 and P2 are always produced. Furthermore, in order to satisfy the constraint of a minimum profit in the worst scenario, as the value of the worst case is more demanding, solutions prefer producing fewer amounts of P3 and P4, because products P1 and P2 have a less uncertain demand than P3 and P4. Limiting the whole problem was solved in approximately 3.8 h CPU time, which implies a great time reduction compared to the rigorous solution procedure by using the ε-constraint method discretizing the space into 12 subintervals. This comparison can be observed in Table 4.

Let us note that for each Pareto solution of the problem a cumulative probability curve can be plotted (i.e., each efficient schedule in terms of expected profit and risk has an associated cumulative probability function). Cumulative risk curves provide further insights for the better understanding and assessment of the trade-off posed between risk and expected profit.[28] Figure 5 represents the cumulative risk curves of the solutions provided by the fixed and flexible recipe strategies for a worst case equal to 9,600 m.u.

The aforementioned curves show the level of financial risk incurred at each profit level. Comparing the curves obtained for the fixed and the flexible recipe framework, one can see how the flexible recipe curve lies entirely above the fixed recipe one. Thus, the flexible recipe framework not only leads to lower probabilities of poor profits, but also to higher chances of large benefits, which makes the overall production less risky in economic terms. Hence, the flexible recipe solution performs better over the entire uncertain space as can be seen in the shift to the right of the risk curve. For instance, a 5% probability of scenarios with earnings below 12,000 m.u. is achieved using flexible recipes, while this probability increases up to 10% using

Table 3. Optimal-Pareto Solutions Applying SAA for the Flexible Recipe Framework

			Number of produced batches			
Solutions	WC, m.u.	Expected Profit, m.u.	P1	P2	P3	P4
1	8280.18	15858.74	3	3	3	3
2	9133.99	15715.05	3	3	2	3
3	9774.14	15285.79	3	3	2	2
4	9811.44	15097.96	3	3	1	3
5	9960.29	14528.82	3	3	2	1

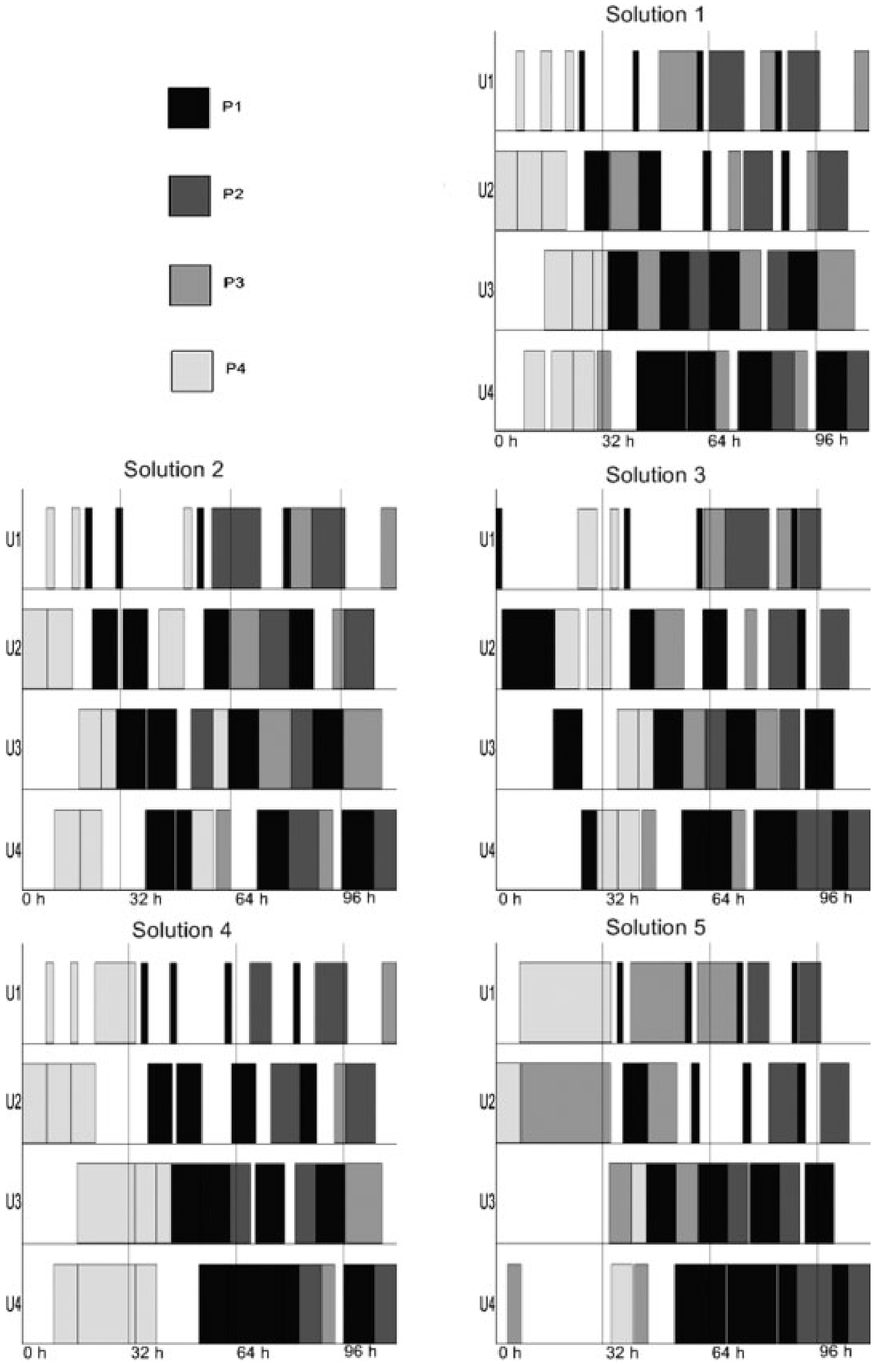

Figure 4. Associated schedules for each solution.

traditional fixed recipes. On the other hand, the use of flexible recipes yields higher probabilities of larger benefits. For instance, a 45% probability of earnings above 16,000 m.u. is reported by this solution compared to the very scarce probability, less than 1%, using fixed recipes. Consequently, this makes the use of flexible recipes a very

Table 4. Computational Results

	Bin., cont., rows	Average CPU, s	Number of realisations	CPU, h
Full problem using fixed recipes	224, 654, 1669	2600	12	8.7
Full problem using flexible recipes	224, 808, 1853	4300	12	14.3
SAA algorithm using flexible recipes	224, 311, 1653	70	100	3.8
	212, 819, 1753	69	100	

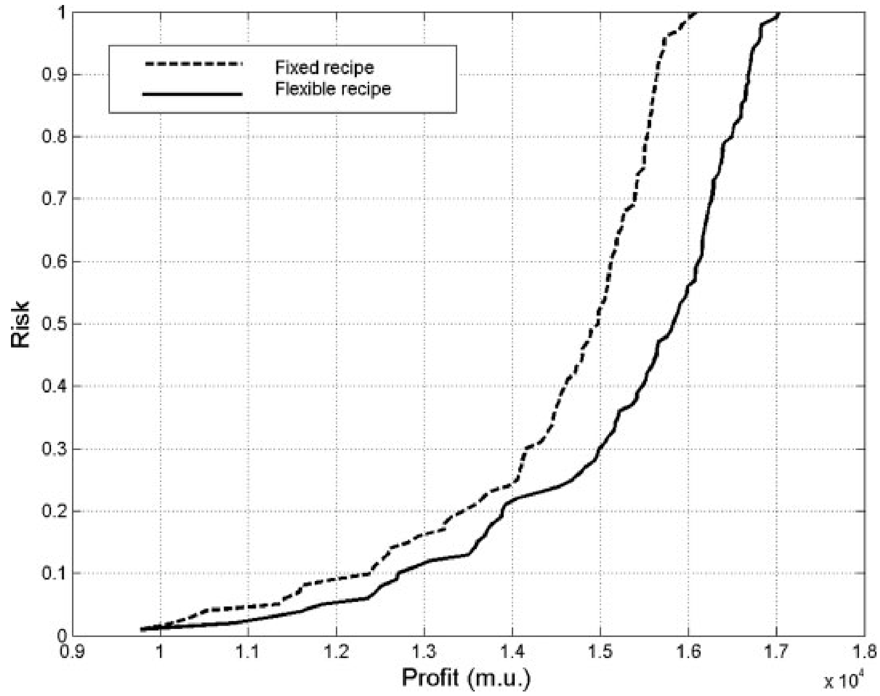

Figure 5. Cumulative risk curve for a worst-case value of 9600 m.u.

attractive alternative given its capacity of properly managing the financial risk.

Conclusions

This article has proposed a novel stochastic mathematical formulation to address risk management in the scheduling problem associated with batch chemical plants operating under demand uncertainty. The main novelty of our work lies in the application of a flexible recipe framework as a way of reducing the probability of meeting unfavorable scenarios in an uncertain market environment. The problem has been mathematically posed as a multiobjective multiscenario two-stage stochastic formulation accounting for the maximization of the profit and the worst case value. The resulting formulation is based on a continuous-time domain representation and the generalized notion of precedence. As such, our model explicitly incorporates the trade-off between risk and profit at the decision-making level. Furthermore, a decomposition strategy, based on the sampling average approximation (SAA) has been studied as a way of overcoming the numerical difficulties associated with the application of the proposed strategy to large-scale industrial scenarios. The decomposition technique provides near optimal solutions, and incurs in much less CPU time than the monolithic formulation.

Finally, the effectiveness of the proposed approach as a decision-making tool has been highlighted through a scheduling case study. Results indicate that for a given level of risk, higher benefits can be obtained by using flexible recipes. Furthermore, using flexible recipes allows attaining conservative solutions that would be impossible to obtain by applying the conventional approach. Therefore, the use of flexible recipes has been shown to be a highly valuable risk management instrument to support the decision making process in an uncertain market environment. Future work will be envisaged to extend and develop this framework by considering new risk control measures using different techniques.

Notation

Subscripts

p, p' = product
i, i' = batch
s, s' = processing stage
p, i, s = task (p,i,s)
u, u' = processing units
f, f' = flexible recipe items and process outputs
e = scenario
$DTOP$ = time duration in the flexible recipe model
DPS = reaction yield in the flexible recipe model
$DTEMP$ = temperature in the flexible recipe model
$DKOH$ = amount of KOH in the flexible recipe model
$DFOR$ = amount of Formaldehyde in the flexible recipe model

Sets

FL_{ps} = stages s of product p with a flexible recipe
FP_{ps} = set of recipe items of the linear flexible model for stage s of product p
I_P = batches of product p
S_P = stages for producing product p
U_{ps} = set of available units for processing product p at stage s
E = scenarios

Parameters

H = scheduling horizon
npt_{ps} = nominal processing time for s-th stage of product p
tt_{ps} = transfer times
s^l_{pi} = last processing stage for batch i of product p
M = a very large number

$lfmod_{psf}$ = linear flexible recipe model coefficient of recipe item f at processing stage s of product p
$fpub_{psf}$ = maximun positive deviation of parameter f from the nominal recipe
$fplp_{psf}$ = maximun negative deviation of parameter f from the nominal recipe
$dcost_{psf}$ = deviation cost from nominal recipe parameters
$prob_e$ = associated probability for each scenario
$mdem_p$ = mean demand for product $_p$
dem_{pe} = demand of product p for scenario e
$demdev_p$ = demand deviation for product p
bsz_p = batch size of every batch of product p
sp_p = batch size of every batch of product
$pinv_p$ = selling price of every batch of product p
pc_p = production costs of a batch of product p
udc_p = unsatisfied demand cost for product p per unit time
mpc_p = maximum plant capacity for producing product p
θ = optimization parameter

Continuous variables

FT_{pis} = completion time for the task (p,i,s)
ST_{pis} = starting time for task (p,i,s)
δ_{pisf} = deviation for task (p,i,s) from nominal recipe value of the flexible parameter f
PFS_e = deterministic profit for scenario e
$E[PFS]$ = expect profit for a set of scenarios
WC = worst case profit
$SALES_{pe}$ = sales of product p in scenario e
IN_p = inventory of product p
$\mathrm{IN}_p^{\mathrm{ini}}$ = initial inventory of product p
QP_p = produced amount of product p

Binary variables

$X_{pisp'i's'}$ = binary variable equals to 1 if task (p,i,s) is processed before another task (p',i',s'), and 0 otherwise
Y_{pisu} = binary variable equals to 1 if stage s bath i of product p is produced and allocated to unit u and 0 otherwise

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