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Exploiting the use of a flexible recipe framework to manage financial risk

Gonzalo Guillén-Gosálbez,^a Sergio Ferrer-Nadal,^b Luis Puigjaner^b

^aDepartment of Chemical Engineering, Carnegie Mellon University, 5000 Forbes Ave, Pittsburgh, PA 15213, USA ^bChemical Engineering Department - CEPIMA, Universitat Politècnica de Catalunya, Av.Diagonal 647, E-08028, Barcelona, Spain, luis.puigjaner@upc.edu

Abstract

This work explores the use of the flexible recipe framework as a manner to manage the risk associated with the operation of batch chemical plants under uncertain market trends. The scheduling problem under uncertainty is mathematically formulated as a multi-objective mixed integer linear problem accounting for the maximization of the expected profit and minimization of risk. A decomposition strategy based on the Sample Average Approximation (SAA) is applied to overcome the numerical difficulties associated with such mathematical formulation.

Keywords: risk management, flexible recipes, stochastic programming.

1. Introduction

Traditionally, in batch processing, a production recipe is defined as the entity that contains all the information concerning the sequence of tasks and operating conditions that must be performed 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 in the design. Then, a flexible

recipe operation may be a suitable way of incorporating systematic recipe adaptations depending on the actual process conditions.

Batch manufacturing plants have also to deal with 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 it has been widely recognized the importance of incorporating uncertainties in the scheduling formulations, most of the models developed so far in the literature are deterministic. Thus, the accuracy of the solutions generated using deterministic models may depend on the degree of uncertainty. Furthermore, stochastic models optimize the total expected performance measure but they usually do not provide any control on its variability over the different scenarios assuming that the decision-maker is risk neutral.

This work aims to provide a quantitative tool based on mixed integer modeling techniques to manage the risk associated with the operation of batch chemical plants under uncertainty. The main novelty of our work lies in the application of a flexible recipe mode of operation as a way to control the variability of the objective function over the different plausible scenarios. The main advantages of our approach are highlighted through a case study, in which a comparison with the traditional fixed recipe mode of operation is carried out.

2. Problem Statement

Given are a set of raw materials, intermediate and final products to be manufactured in a multi-purpose batch chemical plant. Given are also a set of production recipes and prices of final products, which are sold at the end of a given time horizon, the topology of the plant and the cost functions. 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. The problem then consists of finding the scheduling decisions that maximize the total expected profit and minimize risk. The profit is computed over a set of demand scenarios and includes sales revenues, operating costs, inventory costs and unsatisfied demand costs.

3. The mathematical formulation

The scheduling problem under uncertainty with risk management considerations can be mathematically formulated as a multi-objective mixed integer linear problem accounting for the maximization of the expected profit and minimization of risk at different target levels. Some of the constraints of our model are based on the work of Méndez et al. [1] and are not given here due to space limitations. In this model, the binary decision variables are denoted by $X_{pisp'i's'}$, which states the general precedence relation between a pair of tasks,

and Y_{pi} , which equals 1 if bath i of product p is produced and 0 otherwise. The remaining constraints are next described in detail.

3.1. 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 manufacturing stage s of batch i belonging to product p from their nominal values are denoted by the continuous variable δ_{pisf} . In this work, a linear flexible recipe model (constraint 1) has been adopted. Such model is only valid around a flexibility region (see constraint 2).

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

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

3.2. Timing constraints

Constraint 3 establishes the duration of a task taking into account the processing times of the recipe stages and also the time deviations associated with the flexible tasks, while constraint 4 forces all the tasks to be completed within the specified scheduling horizon of length H.

$$FT_{pis} \ge ST_{pis} + npt_{ps} + \delta_{pisDTOP} \qquad \forall p \in P, i \in I_P, s \in S_P$$
(3)

$$FT_{pis} \le H \qquad \forall p \in P, i \in I_P, s \in S_P \tag{4}$$

3.3. Market constraints

Equation 5 states that the sales can be lower or equal to the demand as our model assumes that some of the demand can actually be left unsatisfied because of limited production capacity.

$$SALES_{pe} \le DEM_{pe} \quad \forall p \in P, e \in E$$
 (5)

$$SALES_{pe} \le QP_p \quad \forall p \in P, e \in E$$
 (6)

$$QP_p = \sum_{i \in I_p} \sum_{s \in \{s_p\}} bsz_p Y_{pis} \quad \forall p \in P$$
(7)

Moreover, equation 6 constraints the sales to be lower or equal to the amount produced, which is computed through equation 7. 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 such batches.

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3.4. Objective function

The model must account for the maximization of the expected profit and minimization of risk. The expected profit is computed by calculating the average of profits over the entire range of scenarios (equation 8). The profit values in each scenario are computed assuming 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. It also includes a deviation cost factor that penalizes the positive and negative deviations of every recipe item from the nominal operating conditions.

$$E[PFS] = \sum_{e \in E} prob_e \cdot PFS_e \tag{8}$$

The financial risk associated with a plan under uncertainty (FR_{Ω}) is defined as the probability of not meeting a certain target profit (maximisation) level referred to as Ω [2]. From a mathematical programming point of view, minimizing the financial risk for a continuous range of profit targets results in an infinite multi-objective optimization problem. Even though this model would be able to reflect the decision-maker's intention, it would be computationally prohibitive. However, the ideal infinite optimization can be approximated by a finite multi-objective problem that only minimizes risk at some finite number of T profit targets Ω_t and maximizes at the same time the expected profit (E[PFS]). This approach gives rise to the following finite multi-objective formulation:

$$\max \{E[PFS]; -FR_{\Omega_1}; -FR_{\Omega_2}; \dots; -FR_{\Omega_T}\}$$

Where the financial risk for each target level t is computed through the following constraints:

$$FR_{\Omega_{i}} = \sum_{e} prob_{e} \cdot z_{e\Omega_{i}}$$
(9)

$$\Omega_t - U_e \cdot z_{e\Omega_t} \le PFS_e \le \Omega_t + U_e \cdot (1 - z_{e\Omega_t}) \qquad \forall t, e$$
(10)

Equation 10 is a big-M constraint that forces the new integer variable $z_{e\Omega t}$ to take a value of zero if the profit for scenario *e* is greater or equal than the target level (Ω_t) and a value of one otherwise. Here *Ue* denotes the upper bound of the profit in scenario *e*. The inclusion of these new integer variables represents a major computational limitation of the resulting formulation. To circumvent this problem, we propose to apply in this work a variation of the sample average approximation firstly introduced by [2]. Thus, the original two-stage stochastic problem with *E* scenarios is decomposed into *E* deterministic problems that are

solved for every scenario e in the original formulation. Each solution (i.e., schedule) is then fixed in the original problem and assessed over the entire range of scenarios. The deterministic solutions generated in this way are finally filtered by applying the dominance concept. Thus, if curve A lies entirely above curve B, the former solution is automatically discarded as this means that solution A is dominated by solution B in terms of expected profit and financial risk at the different target levels [2].

4. Case study

The advantages of our framework will be illustrated through the batch-wise production of benzyl alcohol by the crossed-Cannizaro reaction that is carried out in a multi-purpose batch chemical plant. In this work, we use the linear approximation of the flexible recipe model introduced by [3]. Uncertainty in demand and prices of final products is considered through 100 scenarios generated by applying a Monte Carlo sampling. Some extra data of the problem are shown in tables 2 and 3.

Table 2. Problem data

Table 3. Deviation variables

Product	P1	P2	P3	P4	Deviation variables		< Flexibility <		Dev. cost
bsz _p , kg/batch	40	55	40	35	Devia			nonity _	Dev. cost
mpc _p , kg	160	110	120	105	δ_{DPS}	yield	0	0	-
mdem _p , kg	280	110	120	120	δ_{DTEMP}	temperature	-0.7	0.5 °C	0.03 \$
pv _p , \$/batch	70	55	40	40	δ_{DTOP}	duration	-1.25	0.5 h	0.02 \$
rmc _p , \$/batch	8	7	5	8	δ_{DKOH}	Amount of KOH	-27	8.5 g	0.05 \$
pinv _p , \$/h	1	2	1.1	0.5		A			
udc _p , \$/kg	4	3	2	3	δ_{DFOR}	Amount of Formaldehyde	-30	7.5 g	0.04 \$

Thus, 100 schedules are obtained by solving a deterministic problem for every scenario. Each schedule is next evaluated over the entire range of scenarios through the stochastic formulation. Finally, the risk curves associated with each solution are filtered by applying the dominance concept. From the original set of 100 curves, only 8 are non-dominated.

The risk curves associated with these solutions are shown in Figure 1 along with the one corresponding to the "wait and see" solution. Notice that each curve is associated with a certain schedule that behaves in a specific way under the uncertain environment. For instance, schedule 1 reflects a manufacturing strategy that tends to be riskier than the one associated with schedule 3. By inspecting in detail the schedules, not given here due to space limitations, we can see how schedule 3 is producing less batches of P3, which has a very high demand variability, and more batches of P2, the demand of which happens to be less variable.



Figure 1. Set of non-dominated risk curves

5. Conclusions and future work

This work has presented a novel framework to manage the risk associated with the scheduling of batch chemical plants that exploits the use of a flexible recipe framework as a manner to handle uncertainties in demand and prices. The problem has been formulated as a moMILP, the solution of which has been approximated by the sample average approximation (SAA) algorithm. The main advantages of our work have been highlighted through a case study for which a set of solutions appealing to decision makers with different attitudes towards risk has been obtained and a comparison with the traditional non-flexible batch operation mode has been carried out.

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References

- 1. C.A. Méndez and J. Cerdá, Optim. Eng., 4 (2003) 7.
- 2. A. Aseeri and M. Bagajewicz. Comp. and Chem. Eng. 28 (2004), 2791
- 3. J. Romero, A. Espuña, F. Friedler and L. Puigjaner, Ind. Eng. Chem. Res. 42 (2003), 370.