Risk conscious scheduling of batch processes

G. Sand and S. Engell

Process Control Laboratory, Dortmund University, 44221 Dortmund, Germany

Abstract We consider real-time scheduling problems of flexible batch processes under the special consideration of uncertainties. Any decision has to be made subject to a certain risk since it affects the future evolution of the process, which is not precisely predictable. This difficulty can be faced by a moving horizon approach with frequent re-optimisations. We propose the use of a model framework from stochastic programming to reflect the uncertainty and the potential of recourses realistically. The framework is applied to a real-world process from the polymer industries, a decomposition algorithm is sketched and numerical results are given.

Keywords real-time scheduling, flexible batch processes, stochastic integer programming

1. INTRODUCTION

During the operation of flexible batch plants, a large number of discrete decisions has to be made in real time and under significant uncertainties. Any prediction about the evolution of the demands, the availability of processing units and the performance of the processes is necessarily based on incomplete data. Resource assignment decisions must be made at a given point of time despite the fact that their future effects can not be foreseen completely.

The multi-product plant is the most popular flexible plant concept in the chemical industries, especially in the growing market for specialty chemicals, where small volumes of high-valued products in several complicated synthesis steps are produced. Its flexibility enables the production of a variety of products on a single plant and for rapid and cost efficient adaptations of the product supply to the customer demands.

To operate such a flexible plant in a dynamically changing environment, a large number of management decisions and control activities is needed, so efficient process management and control systems have a strong impact on the profitability of the plant. For the problems on the lower control levels, standardized solutions exist, and new plants are often highly automated on these levels.

Nevertheless, the management of process operations, in particular planning and scheduling activities, can hardly be standardized, since these higher-level problems are dominated by complex interactions which are highly plant specific. Therefore, computer-aided planning and scheduling is still a topic of extensive academic research and so far seldom realized in industry. A large number of publications demonstrate that the theory of mathematical programming (MI(N)LP) provides promising methods to model scheduling problems adequately and to solve them efficiently (for an overview see Ref. 1).

An appropriate strategy to schedule highly coupled processes online is based on a moving horizon approach, similar to model predictive control (MPC): The problem is solved for a certain horizon, and the first decisions are applied. Due to modelling inaccuracies or disturbances of the process, the computation must be iterated after some period taking new infor-
mation into account. While this is a “closed loop” strategy with decisions in the feedforward and observations in the feedback branch, the models used are often based on an “open loop” view, which neglects the optimisation potential of re-optimisations subject to feedback information. Undoubtedly, the quality of scheduling decisions can be increased by modelling the uncertain future evolution along with corresponding reactions more realistically.

2. RISK CONSCIOUS MODELLING

2.1. Motivation
In recent years, several publications appeared which address the issue of uncertainty (e.g. Ref. 2-6). However, so far the following essential aspects of uncertainty conscious scheduling models received only little attention:

1. Plant managers who face uncertainty will try to maximize the mean profit but they will also try to avoid the rare occurrence of very unfavourable situations, e.g. heavy losses. Naturally they aim at a compromise between expected profit and accepted risk.

2. In any iteration, only the first few decisions in the horizon are really relevant. Due to temporal couplings, the remainder of the decisions has to be anticipated, but they are never applied since the solution will be modified in the next iteration.

The second aspect cannot be reflected by open loop models since these models do not differentiate between “here and now” and “recourse” decisions. Compensations to possible disturbances can only be considered, if the model reflects different possible scenarios of the process evolution with corresponding degrees of freedom to react to certain realisations.

Concerning the first aspect, the maximum expected profit for a number of possible process evolutions can in general not be determined by calculating the expected evolution and solving an optimisation problem for the mean values. Using a scenario based model usually leads to higher expected profit and provides sensitivity information to control the risk.

2.2. Stochastic integer programming
The mentioned aspects exactly fit into the modelling framework of two-stage stochastic integer programming. For linear models and a scenario-based representation of uncertainties, a deterministic equivalent of a two-stage stochastic integer program (2-SSIP) can be written as a large mixed-integer linear program (MILP):

\[
\begin{align*}
\max_{x, y_1, \ldots, y_\Omega} & \quad c^T x + \sum_{\omega=1}^{\Omega} \pi_\omega q_\omega^T y_\omega \\
\text{s.t.} & \quad T_\omega x + W_\omega y_\omega = h_\omega, \quad x \in X, \quad y_\omega \in Y, \quad \omega = 1, \ldots, \Omega.
\end{align*}
\]  

In this framework the uncertain evolution is represented by a finite number of scenarios \( \omega \) with corresponding probabilities \( \pi_\omega \). The variables are assigned to 1st and 2nd stage vectors \( x \) and \( y_\omega \), which belong to polyhedral sets \( X \) and \( Y \) with integer requirements. The \( x \)-vector represents “here and now”-decisions which are applied regardless of the future evolution. It therefore is identical for all scenarios. In contrast, the \( y_\omega \)-vectors model scenario-dependent recourses under the assumption that the respective scenario materializes. The uncertainties may affect any parameter of the model, such that \( \Omega \) different matrices and right hand sides \( T_\omega, W_\omega \) and \( h_\omega \) may arise. The classical objective is to maximize the first stage profit plus the expected second stage profit computed as a weighted sum of \( x \) and \( y_\omega \) subject to the weighting-vectors \( c \) and \( q_\omega \).
2.3. Risk Aversion

The expected value criterion does not utilize the full information about the shape of the probability distribution of the objective function over the scenarios. This may lead to results with a high expected profit while a few scenarios give very low values of the objective function. To control the risk that the profit falls below a certain threshold \( \varepsilon \), Eq. (1) can be extended by a excess probability:

\[
\max_{x,y_1,\ldots,y_\Omega,u_1,\ldots,u_\Omega} \quad c^T x + \sum_{\omega=1}^{\Omega} \pi^T_{\omega} q_{\omega} y_{\omega} - \delta \sum_{\omega=1}^{\Omega} \pi^T_{\omega} u_{\omega}, \quad s.t. \quad T_{\omega} x + W_{\omega} y_{\omega} = h_{\omega}, \quad c^T x + q^T_{\omega} y_{\omega} \geq \varepsilon - M u_{\omega}, \quad x \in X, \quad y_{\omega} \in Y, \quad u_{\omega} \in \{0,1\}, \quad \omega = 1,\ldots,\Omega.
\]

The idea is to compute the probability that the profit falls below a threshold \( \varepsilon \) by using binary indicator variables \( u_{\omega} \) in a big-M inequality, and to reduce the expected value proportionally. The parameter \( \delta \) weights the risk relative to the mean value. This extension fits into the 2-SSIP framework and increases the model size only marginally.

From the syntactical point of view, any deterministic MILP-model can be regarded as a single-scenario base-model, which can be extended to a 2-SSIP according to Eq. (1) or (2) under two conditions: Firstly, the uncertainty must only affect the parameters and secondly, the decisions must not affect the probabilities. (E.g. models which represent time by an index cannot reflect temporal disturbances.) If these conditions are fulfilled, the scenarios are able to represent any probability distribution, e.g. tree-structured evolution estimations and empirical distributions. It should be noted that even coarsely approximated uncertainty representations have an advantage over mean value representations, since it is mathematically proven that 2-SSIPs lead to better (1st-stage-) scheduling decisions than obtained for the corresponding mean value problems (Ref. 7).

3. A BENCHMARK PROBLEM

The described modelling methodology was applied to a flexible batch process from the polymer industries: The multi-product batch plant shown in Fig. 1 is used to produce two types (A/B) of expandable polystyrene (EPS) in 5 grain size fractions each. The preparation stage and the polymerisation stage are driven in batch mode whereas the finishing is done continuously. A polymerisation batch is produced according to a certain recipe (out of ten possible ones), which determines the EPS-type and the grain size distribution. The resulting mixture of

---

Fig. 1. Flowsheet EPS-process
grain sizes is buffered in one out of two mixing vessels and then continuously fed into the two separation stages, which must be shut down temporarily if a minimal flowrate cannot be maintained.

Scheduling decisions to be made are: 1. choice and 2. timing of the recipes of the polymerisations, 3. outflows of the mixing vessels, and 4. start-up- and shut-down-times of the finishing lines. They are subject to resource constraints and non-linear equality constraints describing the mixing process. The objective is to maximize the profit calculated from revenues for satisfying customer demands in time and costs for polymerisations, start-ups/shut-downs of the finishing lines, inventory, and penalties for demand shortages.

The uncertainties can be classified into endogenous and exogenous uncertainties, which are or are not linked to process events, respectively. Endogenous disturbances comprise polymerisation times and yields; disturbances in the plant capacity and in the demand are regarded to be exogenous in nature.

4. MASTER SCHEDULING MODELS

4.1. The model family

The scheduling problem is decomposed into a detailed scheduling and a master scheduling problem (DS/MS), which are implemented in a cascaded feedback structure (see Ref. 8). A deterministic base model for the DS problem was developed by Schulz (Ref. 9), so in the following we will focus on the master level.

We developed a family of MS base models which comprises several model instances for the process and for the profit. It uses a time representation which is based on three fundamental considerations:

1. The problem is formulated on a finite moving horizon of reasonable length. By shifting the horizon, some of the former recourse decisions \( y_{eo} \) become here and now decisions \( x \). This auto-recourse, i.e. the property, that the same model is used throughout, gives rise to a uniform model structure over the entire horizon.

2. According to its horizon, the MS model reflects uncertainties with long-term effects, i.e. uncertain demands and capacities, which are both exogenous in nature. Since the probability of the occurrence of an exogenous event within a certain period of time depends on the period length, only the consideration of fixed time periods allows for the definition of uncertainty scenarios \( \omega \) with fixed probabilities \( \pi_{eo} \).

3. An appropriate time representation is a multi-period grid with fixed time intervals, and the period lengths have to be chosen such that the probability of a disturbance is significant. Since the need for re-optimisations is determined by the same criterion, the iteration period is synchronous with the time grid. A reasonable choice is a horizon of 14 periods of 2 days each. The first 2 intervals are defined as the 1st stage, they serve as a guideline for the DS level.

4.2. Illustrative instances

To give an impression of the models we present the key ideas by some illustrative constraints and refer to Refs. 8, 10 for more details.

Scheduling decisions to be made on the master level are 1. the rough timing of start-ups/shut-downs of the finishing lines, 2. the rough timing of polymerisations and 3. the assignment of recipes. Given \( I \) fixed time periods \( i \), the degrees of freedom are represented by the variables \( z_{ip} \in \{0,1\} \) and \( N_{irp} \in \mathbb{N} \), which represent the operation mode of the finishing line \( p \) in \( i \) and the number of polymerisation starts according to recipe \( r_p \in \{1, \ldots, R_p\} \) in \( i \), re-
spectively. The relevant constraints are the capacity of the polymerisation stage and of the finishing lines. It turned out that the interaction between the periods is of major importance.

Considering the constraint for minimal throughput of the finishing lines, the formulation for decoupled periods would read as follows (\( C \) - mixer levels, \( F \) - feed rates, min – minimum, max – maximum, 0 – initial state):

\[
\sum_{r_p=1}^{R_p} N_{i r_p} \geq C^\min_p + z_{i p} F^\min_p \quad \forall i, p. \tag{3}
\]

The technique to model the couplings is to constrain sums of periods (the non-linearity can exactly be linearized):

\[
\sum_{i'=i}^{i} \sum_{r_p=1}^{R_p} N_{i' r_p} \geq z_{i' r_p} z_{(r+1)_p} C^\min_p - \begin{cases} C^0_p \text{ if } i = 1 \\ z_{(i-1)_p} z_{i p} C^\max_p \text{ else} \end{cases} + \sum_{i'=i}^{i} z_{i' p} F^\min_p \quad \forall i, i', p | i \leq i'. \tag{4}
\]

The use of Eq. (3) instead of Eq. (4) leads to more shut down-procedures if a finishing line is driven at its lower capacity limit and to significantly higher costs.

An essential target of profit oriented scheduling is to maximize the sales subject to demand and supply constraints. With \( M_{i f_p} \in IR_+ \) denoting the sales of product \( f_p \) in \( i \), \( B_{i f_p} \in IR_+ \) the demand and \( p_{f_p r_p} \in IR_+ \) the yield of \( f_p \) according to a certain recipe \( r_p \), Eq. (5) defines the demand and the supply constraints, respectively:

\[
\sum_{i'=1}^{i} M_{i' f_p} \leq \sum_{i'=1}^{i} B_{i' f_p} \quad \wedge \quad \sum_{i'=1}^{i} M_{i' f_p} \leq \sum_{i'=1}^{i} \sum_{r_p} p_{f_p r_p} N_{i' r_p} \quad \forall i, f_p, p. \tag{5}
\]

A disadvantage of this formulation is the missing distinction between timely and late sales. To control the lateness, an index \( d \) represents delay intervals; the constraints then read as follows:

\[
\sum_{d} M_{d(i+d-1)f_p} \leq B_{i f_p} \quad \wedge \quad \sum_{j=1}^{i} \sum_{d=1}^{j} M_{d f_p} \leq \sum_{j=1}^{i} \sum_{r_p} p_{f_p r_p} N_{j r_p} \quad \forall i, f_p, p. \tag{6}
\]

5. SOLUTION ALGORITHM

The 2-SSIP according to Eq. (1) exhibits the characteristic block-angular matrix structure shown in Fig. 2, left. It may be transformed equivalently by introducing additional vectors \( x_0 \) for any scenario \( \omega \) as well as equality constraints \( x_1 = \ldots = x_\Omega \) represented by \( H \).

The 2-SSIP is solved by a decomposition algorithm (Ref. 11) which exploits the characteristic matrix structure. It is based on a Lagrangian relaxation of the \( H \)-constraints, which are reinforced by a branch and bound-algorithm. At any node of the tree \( \Omega \) scenario-problems are solved by CPLEX, a feasible solution is guessed by heuristics and a bound is generated by solving a Lagrange dual problem with NOA.

Since the various base models exhibit a similar numerical performance extensive numerical studies were performed on the stochastic model instance characterised by Eq. (4) and (5).
The uncertainty was represented by $\Omega = 1,000$ randomly generated rhs-scenarios for the demand and the capacity, such that a 2-SSIP with 140,022 integer variables, 448,000 continuous variables and 736,009 constraints results.

It was solved on a SUN Ultra Enterprise 450 with a 300 MHz processor, and the CPU-time was limited to 4 hours, which is “short” compared to the periods. The algorithm generated solutions with optimality gaps of 5.9 %, and with an additional problem specific pre-processing they were reduced to 4.2 %. The inclusions of the excess probability leads to reductions of risk by 20 % while the expectation value is only changed by 2 % and the numerical performance remains essentially unaffected (Ref. 10).

6. CONCLUSIONS

The proposed scheduling methodology allows for a realistic representation of future re-optimisations and evolutions with various probabilities within a closed-loop structure. The scenario representation of uncertainty ensures the practical applicability since open-loop models can be extended in principle and empirical probability distributions can be utilized.

Furthermore the efficiency of the approach could be improved in two ways: Firstly, the two-stage program may be extended to a multi-stage program, which takes multiple re-optimisations into account. And secondly, the algorithm implementation may be parallelised on both the stochastic decomposition and the scenario level.

REFERENCES