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Integrating process dynamics within batch process scheduling via mixed-integer dynamic optimization

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HIGHLIGHTS

- Predicted optimal operating conditions not be the best for production requirements.
- Development of tools to fully integrate process dynamics into batch scheduling.
- Integration of operational and scheduling decisions for significant economic savings.

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ABSTRACT

During batch process scheduling, products' batch size, processing conditions as well as operating times are usually established offline and considered out of the scope of the decision making stage. In practice, process dynamics may vary from the ones forecasted, in such a manner that the predicted optimal conditions will not be the best in practice. As a result of this mismatch, the plant usually operates under sub-optimal conditions, but if the process is flexible, its processing conditions can still be adapted to the actual plant needs in order to improve the overall performance. Given this situation, there is a strong motivation for developing models and optimization tools to fully integrate process dynamics into batch scheduling. In this work, the potential of directly including control variables with time varying values and variable batch sizes in the scheduling of batch plants is explored. The optimization of process dynamics, which is time varying, along with scheduling tasks is accomplished using rigorous mixed-integer dynamic optimization techniques. Through several examples, we show that integrating both decision-making levels can lead to significant economic savings.

1. Introduction

The need for improved models and tools to integrate the scheduling function with the optimization of process dynamics has gained wider interest in the recent past. Despite the potential benefits of such integration, which have been already acknowledged in the literature (Chatzidoukas et al., 2003; Nystrom et al., 2005; Terrazas-Moreno et al., 2007; Prata et al., 2008), little work has been conducted concerning the full integration of process models within scheduling formulations for general batch processes.

One of the very first works to consider the integration of process dynamics in the batch scheduling problem was presented by Bhatia and Biegler (1996). These authors developed models for the design and scheduling of a very specific type of batch process (i.e., flowshop plants with unlimited intermediate storage and zero wait transfer policies with one unit per stage) that integrated dynamic aspects. In their work, processing decisions were resolved by discretizing the dynamic process models through collocation on finite elements. Numerical examples showed that dynamic process considerations can contribute significantly to increase profitability. Their work was further extended to deal with product and plant uncertainty (Bhatia and Biegler, 1997).

On the other hand, Mishra et al. (2005) broadly classify the scheduling problem formulation into two categories: standard recipe approach and overall optimization approach. The former comprises two steps: a recipe is defined in the first step (either empirically or by single batch optimization), while in the second step, the scheduling problem is posed on the basis of these standardized recipes. The overall optimization approach (direct approach) includes the process dynamics in the scheduling problem. This consideration increases the degrees of freedom of the standalone scheduling model, providing more flexibility to the optimization and ultimately yielding better solutions.

Recently, Nie et al. (2012) propose a systematic approach that applies to the integration of scheduling and dynamic optimization, by posing a mixed-logic dynamic optimization problem, which is further transformed in a MINLP problem. They apply their formulation to a flowshop and a jopshop examples. However, they consider the state

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equipment network formulation under the assumption of unlimited intermediate storage conditions. Thus, they compare the traditional recipe and process dynamics case but do not propose any other intermediate approach.

All previous works which addressed the integration of process dynamics into batch scheduling embedded the dynamic characteristics of the specific process into the scheduling formulation and considered either cyclic scheduling, small sized short-term scheduling problems with specific process dynamics for all batches of a given product or unlimited intermediate storage policies. Therefore, they were restricted to very specific batch facilities. In this work, the scope of previous works is enlarged by proposing a general approach for the short-term scheduling of batch plants that explicitly accounts for the process dynamics, and includes the possibility for different batch process dynamics for a given product under unlimited and zero wait storage policies. Thus, an intermediate approach which considers process dynamics indirectly as polynomial approximation in the scheduling problem is studied. The dynamic optimization problem is discretized by means of a simultaneous discretization method, namely the orthogonal collocation method over finite elements (Bhatia and Biegler, 1996; Mishra et al., 2005), resulting in a nonlinear problem (NLP). Even more, the application of this technique in the context of a scheduling problem, which contains integer variables, gives rise to a mixed integer nonlinear programming (MINLP) formulation which can be solved via standard MINLP solution algorithms. Several examples are employed to illustrate the benefits of such proposed approach as compared with the use of traditional fixed recipes and approximations based on polynomials.

2. Problem statement

In order to improve the overall plant performance, this work considers full process dynamics at the scheduling level and focuses on the optimization of dynamic control variables as well as proper scheduling ones. The problem of interest can be formally stated as follows:

Given:
Process dynamics:

- a set of control variables, such as temperature, feed flows or pressure, which may be time variable;
- a dynamic process model of each process operation, which establishes the relationship between process state variables and control variables;
- a set of constraints imposed on the process dynamics.

Process operations planning data:

- a specific time horizon;
- a set of materials: intermediate and final products, and raw materials, and their corresponding management constraints: time availability, storage policy, etc.;
- a set of expected final products with minimum and maximum demands;
- a fixed batch plant topology with a set of available equipment units for each processing stage;
- a set of production recipes establishing specific process dynamics and stage sequences;
- a set of production stages which may be either (i) fixed: processing times, mass balance coefficients and resources utilization are optimized and assigned beforehand, or (ii) variable: defined by the corresponding process dynamics.

Economic data:

- the expected selling price for every final product;
- a model for production cost assessment regarding issues such as labor, energy, raw material and unfulfilled demand costs, and their corresponding parameters;
- a set of environmental, quality or safety constraints that have an associated economic cost.

The goal is to determine:

- the number of batches required to meet the demand and their corresponding batch size;
- the assignment and sequencing of the batches;
- the amount of final products to be sold;
- the processing times of the variable stages of each batch;
- the operating condition profiles for each of the control variables associated to the production stages of each batch;
- the dynamic response of the process.

that optimize the adopted performance metrics. An economic objective function is used to assess the overall plant performance at both the scheduling and control levels. Particularly, two economic indicators, namely profit (Eq. (1)) and profitability (Eq. (2)), will be used as objective functions. Profit is determined from the revenues, operating costs (such as electricity, raw materials, steam or water consumption) and unfulfilled demand penalty. As a result, the scheduling and process dynamic decisions are translated into economic terms (as expressed in the formulation section), resulting in a practical and straight-forward measure of the overall performance:

$$z^{profit} = Revenues - OperatingCost - DemandPenalty \tag{1}$$

$$z^{profitability} = \frac{z^{profit}}{z^{Mk}} \tag{2}$$

For designing the fixed recipes, the profitability measure (Eq. (2), z^{Mk} being the production makespan) is used as objective function.

3. Methodology

The scheduling task accounting for process dynamics is posed in mathematical terms as a mixed-integer dynamic optimization (MIDO) problem. The dynamic models of the recipe operations may give rise to a system of ordinary differential equations (ODE). These ODEs are discretized prior to being combined with the scheduling formulation. The following subsections describe how the MIDO problem is constructed.

3.1. Step 1: dynamic model considerations

The most applied techniques to solve dynamic optimization problems are the direct sequential and simultaneous dynamic optimization methods, according to explicit or implicit integration of the dynamic equations. Since decision variables, u, may depend on time and so have infinite dimensions, they must be parametrized to a finite number of parameters in order to use numerical techniques. The sequential approximation method applies the optimization only to the control variables, and the differential equations are integrated by means of standard integration algorithms. Therefore, at every step of the optimization process the differential equations are satisfied. Thus, it is a method which tends to be slow, specially if there are inequality constraints, and the solution quality strongly depends on the parametrization of the control profile. Regarding simultaneous approaches, they avoid the explicit integration of the control variables, and the