Integrated Scheduling and Control of Continuous Multi-product Plants with Product-dependent Processing Sequences

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Abstract

A modeling and optimization framework is presented for the simultaneous scheduling and control of continuous multi-product plants. The recipes for the manufactured products differ not only in the raw materials fed to the first unit of the process, but also in the sequence of processing steps and their operation to reflect the requirements of a certain product. Besides the product specifications, the framework incorporates a process model to predict process dynamics including logical constraints to fix the flowsheet structure as well as the schedule of the products. The resulting mixed-integer dynamic optimization problem is solved via a late discretization approach. The proposed modeling and optimization framework is applied to a simple case study. The flowsheet is representative for fine chemicals production; it consists of three continuous stirred tank and two tubular reactors operated in series. The process structure and the operating conditions are adjusted to meet the requirements of every product.

Keywords: mixed-integer dynamic optimization, continuous multi-product plants, scheduling, optimal control

1. Introduction

Continuous multi-product plants get increasing attention in the specialty chemicals and pharmaceutical industries due to their flexibility and the expectedly high economical potential (e.g. Calabrese et al. (2011)). The integrated scheduling and control of such plants by dynamic optimization remains a technically challenging task of industrial relevance. The dynamic optimization of multi-product plants has largely been restricted to a single reactor or a fixed flowsheet for the production of a single product. In particular, Flores et al. (2006), Prata et al. (2008) and Terrazas et al. (2008) considered continuous stirred tank reactors (CSTR) and Flores et al. (2010) considered a tubular reactor (TR) with different polymerization chemistries and production schedules. While the unit operations as well as the processing sequence are typically switched in case of multi-purpose batch plants (e.g. Kim et al. (2000)), the switching of the flowsheet and the processing sequence in a continuous multi-product process as part of decision making has not been included in integrated scheduling and control frameworks yet. The challenges of designing such flexible continuous multi-product processes include (i) the modeling of the product-dependent processing sequence, (ii) the deactivation of a process unit in case of disuse, and (iii) its reactivation in case of reuse. In this contribution, the considered problem class is described first in Section 2. Then, the modeling framework is presented in Section 3 by means of a CSTR. Section 4 shows how the proposed modeling framework can be applied to a simple case study provided
by Bayer Technology Services (BTS), Leverkusen, Germany. Conclusions are given in Section 5.

2. Problem Class

The type of continuous multi-product plants investigated in this contribution is exemplarily shown in Fig. 1 from different perspectives. Let \( P \) denote the set of products potentially manufactured in the plant. The flowsheet of the multi-product plants consists of a sequence of units arranged in series (Figure 1b) which are denoted by the set \( U \). \( U'_p \subset U \) refers to the set of units with a bypass and a rinsing system (as for example unit 3 in Fig. 1b) needed for manufacturing \( p \in P \). Such a unit \( u \in \bigcup_{p \in P} U'_p \) is shown in more detail in Fig. 1c. The bypass is activated, if a unit is not required for manufacturing product \( p \in P \). Alternative processing sequences which can be realized in the plant in Fig. 1b, are depicted in Fig. 1a. A unit \( u \in U \setminus \bigcup_{p \in P} U'_p \) without bypass and rinsing system (as for example unit 4 in Fig. 1b) is required in the recipes of all products and is therefore operated permanently. Let \( E_u \) and \( S_u \) denote the sets of reagents and solvents which are fed to the multi-product process at unit \( u \in U \). Each reactant \( i \in E_u \) fed to unit \( u \in U \) in solution of some \( j \in S_u \). \( C_{u,in} \) contains all intermediate substances fed to unit \( u \) from the previous unit \( u-1 \). Accordingly \( C_{u,out} \) defines the set of all substances leaving unit \( u \). \( C_{u,by} \) collects all substances leaving unit \( u \) for unit \( u+1 \) (cf. Fig. 1c for notation). Both \( C_{u,in} \) and \( C_{u,by} \) contain the reactants in the set \( E_u \), their respective solvents in the set \( S_u \), the feed components \( C_{u,in} \) and the reaction products generated in unit \( u \). Note, that \( P \subseteq C_{u,by} \) with \( u = \bigcup U \) referring to the last unit in the process flowsheet.

![Figure 1: Process class: (a) processing sequences, (b) the overall flowsheet and (c) a single unit with bypass and rinsing system](image-url)

The multi-stage modeling approach presented by Oldenburg et al. (2008) is adopted here. If a product \( p \in P \) is manufactured in stage \( k \in K \) the binary \( y_{k,p} \) is true; if a product changeover is performed, one of the binaries \( w_{k,p} \), \( p \in P \) is true; thus, \( \vee_{p \in P} (w_{k,p} \vee y_{k,p}) = 1, \forall k \in K \) has to hold. If a changeover to \( p \in P \) is performed, \( p \) is manufactured in stage \( k+1 \): \( w_{k,p} \Rightarrow y_{k+1,p}, \forall p \in P, k \in K \). If a unit \( u \in U'_p \setminus U'_q \) is
operated to manufacture \( p \in P \) in stage \( k \) and is deactivated at the final time \( t_f \) of stage \( k \) in favor of a product changeover to \( q \in P, p \neq q \), in stage \( k+1 \), it is cleaned in isolation parallel to production during stage \( k+1 \) indicated by the binary \( a_{p,k+1,u} \) being true. To rinse unit \( u \in \bigcup_{p \in P} U^*_p \), a cleaning solvent \( i^*_p \in S_u \) is introduced as shown in Fig. 1c. A unit \( u \in \bigcup_{p \in P} U^*_p \) is said to be clean, if a prespecified concentration of the cleaning solvent \( i^*_p \) is attained. All feed streams \( n_{k,u,i,in} \in E_u \cup S_u, \forall u \in U \), binaries and final times \( t_f \) are control variables of the process.

3. Modeling Framework

3.1. Process modeling

On the flowsheet level, the units \( u \in U \) are connected to each other by setting \( n_{k,u,i,in} = n_{k,u,i,in}, \forall i \in C_{u,in}, \forall u \in U \setminus \{i\}, \forall k \in K \) to reflect the processing sequence in the flowsheet. The models for each unit \( u \in U \) determine the outlet streams \( \dot{n}_{k,u,i,out} \in C_{u,out} \). Assuming CSTR units for simplicity, the model is as follows:

\[
\dot{n}_{k,u,i} = (1 - b_{k,u}) \cdot n_{k,u,i,in} - n_{k,u,i,out} + \sum_{i \neq j \in C_{u,in}} n_{k,u,i,in} - n_{k,u,i,out} + \Gamma_{k,u,i} \cdot \forall i \in C_{u,out} (1),
\]

\[
\dot{n}_{k,u,i} = (1 - b_{k,u}) \cdot n_{k,u,i,in} + \bar{n}_{k,u,i,in} - n_{k,u,i,out} + \Gamma_{k,u,i} \cdot \forall i \in C_{u,out} (2),
\]

\[
x_{k,u,i} = n_{k,u,i}/n_{k,u,i} \cdot \forall i \in C_{u,out} (3),
\]

\[
n_{k,u,i,in} = (1 - b_{k,u}) \cdot \sum_{i \neq j \in C_{u,in}} n_{k,u,i,in} + \bar{n}_{k,u,i,in} + \Gamma_{k,u,i} \cdot \forall i \in C_{u,out} (4),
\]

\[
m_{k,u,i,in} = (1 - b_{k,u}) \cdot \sum_{i \neq j \in C_{u,in}} M_{i} \cdot n_{k,u,i,in} + \bar{n}_{k,u,i,in} \cdot M_{i} \cdot \forall i \in C_{u,out} (5),
\]

The amount of substances \( i \) in unit \( u \), denoted by \( n_{k,u,i} \), are calculated from material balances (1) and (3). \( \Gamma_{k,u,i} \) refers to the reaction sink/source of substance \( i \). The molar fraction \( x_{k,u,i} \) of substance \( i \) is defined by Eq. (4) using the total amount of substances \( n_{k,u} \) (cp. Eq. (2)). The outlet streams \( n_{k,u,i,out} \) are calculated by \( n_{k,u,i,out} = n_{k,u,i,out}, \forall i \in C_{u,out} (9) \). The total outlet stream \( n_{k,u,out} \) is determined by Eq. (6), involving the average molar mass \( \overline{M}_{k,u} \) as defined in Eq. (8) and the total mass inflow \( m_{k,u,in} \) determined in Eq. (7). \( M_i \) refers to the molar mass of substance \( i \). If the bypass is activated, i.e., if \( b_{k,u} = 1 \), all feeds \( n_{k,u,i,in}, i \in C_{u,in} \cup U^*_u, \forall u \in U \) except \( \bar{n}_{k,u,i,in} \), the one of the cleaning solvent \( i^*_p \) do not influence \( n_{k,u,i} \), because they are bypassed to \( n_{k,u,i,out}, i \in C_{u,out} \) (Eq. (5)). The outlet streams \( n_{k,u,i,out}, i \in C_{u,out} \) leave the process via the rinsing discharge (cf. Fig. 1c) and the total mass inflow \( m_{k,u,in} \) is determined by the cleaning solvent only. If a unit \( u \) is used in stage \( k \), i.e. if \( b_{k,u} = 0 \), \( m_{k,u,in} \) is calculated from all feed rates and the outlet flow of the unit is calculated from the material balances. The dynamics of units \( u \in U \setminus \bigcup_{p \in P} U^*_p \) is described by Eqs. (1-9) result for \( b = 0 \). During each stage the bypasses of all unneeded units are active: \( w_{k,u} \setminus y_{k,u} \Leftrightarrow b_{k,u} \forall u \in \bigcup_{q \in P} U^*_q \setminus U^*_p \). All differential variables \( n_{k,u,i} \) are
3.2. Variable specifications

Since a reactant \( i \in E_u \) is fed to the unit dissolved in solvent \( j \in S_u \), the feed of this solvent is bounded from below by a constant fraction \( f_{i,j} \) of the feed of reactant \( i \), i.e.,
\[
\begin{align*}
\sum_{j \in S_u} t_{i,j} \cdot f_{i,j} &\geq \sum_{j \in S_u} t_{i,j} \cdot \frac{n_{k,u,i}}{V_u} \cdot f_{i,j},
\end{align*}
\]
Moreover the feed \( \bar{n}_{k,u,i,j,m} \) of the cleaning solvent is nonvanishing only if unit \( u \in U^*_p \) is cleaned during stage \( k \), i.e.,
\[
\begin{align*}
n_{k,u,i,j,m} &\leq \hat{M} \cdot a p_{k,u},
\end{align*}
\]
with \( \hat{M} \) being a sufficiently large constant. The products \( p \in P \) are specified by simple bounds \( l_{p} \leq u_{p} \leq u_{p} \), on the concentrations \( c_{k,u,i,j} \), calculated by \( c_{k,u,i,j} = n_{k,u,i,j} \cdot f_{i,j} \) using the volume \( V_u \) of unit \( u \). Thus the following constraints \( l_{p} \leq u_{p} \leq u_{p} \cdot (1 - y_{k,p} - w_{k,p}) \) have to hold \( \forall q \in P, p \neq q \) during a production phase or at the final time of a changeover phase (i.e. \( y_{k,p} \) or \( w_{k,p} \) are true for \( p \in P \)) using sufficiently large constants \( M \) and \( N \). To specify a clean unit \( u \in U^*_p \) at the final time of a cleaning stage \( k \), the additional endpoint constraint
\[
\begin{align*}
n_{k,u,i,j,m} &\leq g_{u,i,j,m} \cdot n_{i,j,m} - n_{i,j,m} \cdot (1 - a p_{k,u})
\end{align*}
\]
with \( g_{u,i,j,m} \) and the maximal possible amount of substance \( n_{i,j,m} \) of solvent \( i \) in unit \( u \).

3.3. Objective function

The goal is to minimize the costs of consumed raw materials \( i \in E_u \cup S_u \cup \{x_1, \ldots, x_n \} \forall u \in U : 
\[
\begin{align*}
o(t_k) &\equiv \sum_{k \in K} \sum_{i \in E_u \cup S_u \cup \{x_1, \ldots, x_n \}} C_i \cdot n_{k,u,i,j,m} + \sum_{i \in E_u \cup S_u \cup \{x_1, \ldots, x_n \}, j \in S_u} C_i \cdot n_{k,u,i,j,m}.
\end{align*}
\]
For each stage, the total costs comprise the costs of reactant and solvents \( i \in E_u \cup S_u \) (first sum) and the costs of the cleaning solvents (second sum).

4. Case Study

The case study deals with a multi-product plant consisting of 3 continuous stirred tank reactors, 2 tubular reactors and 3 storage tanks for each of the three products, all-in-all about 1500 model equations. The processing steps comprise a lithiation reaction, a coupling reaction, a nitration reaction, a hydrogenation reaction and an activation reaction. The lithiation and nitration reactions take place in a TR, all other reactions take place in a CSTR. The hydrogenation reaction is not required for the manufacturing of the two products \( P_2 \) and \( P_3 \). All reactors are assumed to be operated isothermally. The problem formulation involves seven stages: even stage indices refer to production and odd stage indices to transition stages. In the last stage, a changeover to the product manufactured in the second stage is performed to allow a cyclic production. There are 18 continuous control variables \( n_{k,u,i,j,m} \in U_{out} \cup (E_u \cup S_u \cup \{x_1, \ldots, x_n \} \} each discretized by two piecewise-constant functions on each stage. Further degrees of freedom are the continuous final times \( t_k^f \) of all stages and all the binary variables. The optimization problem has been solved by means of DyOS, a dynamic optimization software developed at the laboratory, which uses late discretization (single shooting) for solving
the continuous optimization problems and a branch and bound method to manage discrete decisions.

The optimal production sequence is 1-2-3. The respective cost function is 5038 Euro and is between 55 and 265 Euro lower than for other sequences. Depending on the starting values, the computing time is up to about 5 hours for each Branch & Bound node. As shown in Figure 2 (left side), the grade specifications with $u_b \leq 0.01$ and $l_b \geq 0.17 \forall p \in P$ hold. The optimal inflow feed rate of the educts $A_1$, $A_2$ and $A_3$ are shown in Figure 2 (right side).

Figure 2: Results of the case study for the production sequence 1-2-3: control profiles of feed inflows (right side), quality of the products (left side)

5. Conclusions

Some or all of the units arranged in a sequence in the flowsheet can be bypassed and cleaned if they are not required to manufacture some product. Future work has to address longer production horizons, extended dynamics for example including energy balances and the bypass modeling of other types of reactors.

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