

Facing New Products Demand through Simultaneous Structural and Operational Decisions in the Design of the Control Recipe

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This work tackles the capacity of adapting batch processes to include new production requirements and plant policies at the operational level. Specifically, procedural models with simultaneous structural and operational decisions are solved to introduce new product manufacturing in given process cells. Global and sustainable performance objectives, such as energy minimization targets, may be used as decision criteria to obtain optimal solutions. The problem is formulated as a mixed-logic dynamic optimization (MLDO), later it is translated to a mixed-integer dynamic optimization (MIDO) and it is solved through a direct-simultaneous approach. The Denbigh Reaction case study is addressed where systematic design of optimal procedural models for new products is performed. The additional degrees of freedom obtained from the joint consideration of structural and operational decisions within the enterprise allow process cell adaptability according to an energy consumption minimization objective.

1. Introduction

Chemical plants management is currently facing a highly competitive framework, which demands not only effective and efficient production to be economically profitable, but also sustainable and environmentally benign manufacturing policies (Kravanja, 2010). Process systems engineering (PSE) community stands out several actuation lines which can be a solution to ensure global optimality in plant management and design problems. The main objective consists of the holistic treatment of the process systems problem, and the integration of different formulations in the lifecycle across multiple scales of chemical spatial and temporal resolution (Klatt and Marquardt, 2009). For instance, integration of process synthesis and operational support system could guarantee a fully functional and optimally operated process plants in the nominal regimes and changing frameworks. The classical approach firstly focuses in plant design and synthesis to perform afterwards process control for attenuating disturbances and maintaining the plant at its desired steady-state. The future process operation must be able to exploit the environmental dynamics, which is mainly caused by changing market conditions and the evolving industry, towards more sustainable production strategies.

Regarding the abovementioned, the integrative direction should be assessed. In this way, model-based systems engineering tools have been promoted, since they present

asset characteristics to deal with chemical processes complexity and multi-objective requirements of decision-making (Klatt and Marquardt, 2009). Particularly, an extended approach in the literature which has generated a lot of scientific interest is the use of logic-based mathematical programming tools to solve process synthesis problems (Raman and Grossmann, 1991) with either algebraic or dynamic process models. However, most of the derived applications are related to continuously operated plants. Process synthesis related to batch processes is refereed in the review by Barbosa-Póvoa (2007). Nonetheless, none of the studies include detailed batch unit operation and process dynamics. On the one hand, research in batch processes design has been mainly focused on equipment sizing, synthesis and scheduling, all of them based on linear models relating investment cost, equipment dimension and capacity and solved using mixed-integer programs (MIP). On the other hand, the field of optimal control has dealt with optimal dynamic profiles in batch processing units (Srinivasan et al., 2003), which has undergone a big expansion in last years. However, only isolated processing units have been considered.

In this context, this work aims to tackle integrated synthesis and operation optimization of batch process cells according to sustainability driving factors, namely energy minimization. Inherent batch processes adaptability is exploited to deal with a changing manufacturing framework, such as the introduction of new products in a production line. In particular, process cell configuration, batch stage times and actuation variable profiles are given as degrees of freedom, and allow for the optimization of the procedural model, also known as control recipe, in a process cell. The proposed resolution approach is an extension of mixed-logic dynamic optimization (MLDO) by Oldenburg et al. (2003), originally used to optimize batch processing units with structural decisions, and broadened in this work to consider several units in a process cell in order to address a multi-level problem.

2. Proposed approach

2.1 Problem statement

This work considers simultaneous structural and operational decision-making for the adjustment of the procedural model within a process cell when new products are considered and a production strategy for energy minimization is tackled. The solution is obtained according to a given production framework defined by: (i) process cell structure (i.e. superstructure and allowable subsystems), (ii) process dynamics (i.e. dynamic model and kinetic data) and (iii) process operations planning data (i.e. demanded products, batch sizes and maximum time horizon). Resulting structural decisions include optimal configurations of the process cell, active equipment pieces and their connectivity and operation mode. Besides, operational decisions refer to processing stages and times, as well as to set-points for actuation variables along time. All of them constitute the optimal control recipe for a specific batch, which is optimized such that energy consumption is minimized.

2.2 Mathematical model

Several types of information should be modeled to solve the previously defined problem, as shown in Figure 1. The process cell superstructure and equipment modes

are formulated using general disjunctive programming (GDP) (Raman and Grossmann, 1994), composed by Booleans, disjunctive equations and logic propositions. Besides, batch operation and process dynamics are modeled with general discrete-continuous models (Vassiliadis et al., 1994), which include differential-algebraic equation (DAE) systems, path and end-point constraints and stage to stage matching functions. The obtained problem is a mixed-logic dynamic optimization (MLDO) problem (Oldenburg et al., 2003), with the simplified form in Eq. 1, where $x \in \mathbb{R}^{n_x}$ and $u \in \mathbb{R}^{n_u}$ are process and actuation variables respectively, $Y \in \{true, false\}^{n_Y}$ are Boolean variables representing structural decisions and t^f is the batch final time. Discrete-continuous model equations are denoted by f , g_i and h_i , which are hold either globally or inside each disjunction term. Finally, function Ω represents logic propositions. Further details regarding batch stages and transitions formulation can be found in Oldenburg et al. (2003).

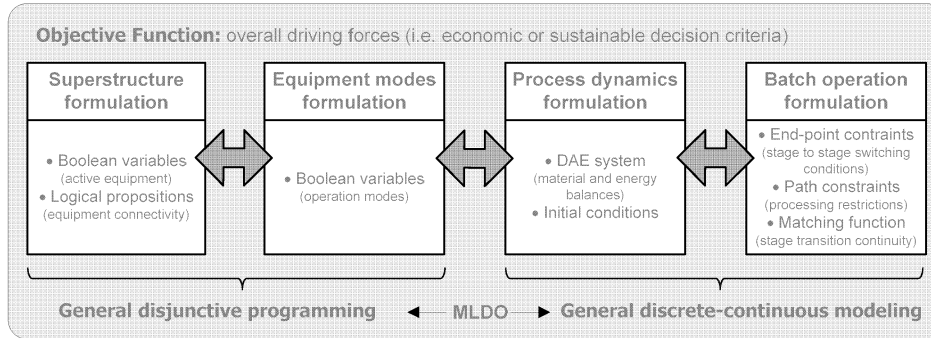


Figure 1: Information required to formulate batch procedural models with operational and structural decisions within a process cell.

$$\begin{aligned}
 \min_{u(t), t^f, Y} \quad & Z = \sum_i b_i + z(x(t^f), t^f) \\
 \text{s.t.} \quad & f(\dot{x}(t), x(t), u(t), t^f) \leq 0, \quad x(0) = x_0 \\
 & \left[\begin{array}{c} Y_i \\ g_i(\dot{x}(t), x(t), u(t), t^f) \leq 0 \\ b_i = \gamma_i \end{array} \right] \vee \left[\begin{array}{c} -Y_i \\ h_i(\dot{x}(t), x(t), u(t), t^f) \leq 0 \\ b_i = 0 \end{array} \right] \quad \forall i \in SD \\
 & \Omega(Y) = true
 \end{aligned} \tag{1}$$

2.3 Resolution tools

Different resolution approaches exist to solve MLDO problems, either based on logical searchers or on the transformation of the logic-based models in integer-based ones. The latter case is used in this work, being the MLDO firstly reformulated as a mixed-integer dynamic optimization (MIDO) problem by replacing the Boolean variables by binaries, logical propositions by algebraic equations and disjunctions by big-M relaxations (Raman and Grossmann, 1991). Then, the obtained MIDO problem is solved using direct-simultaneous approach (Neuman and Sen, 1973) by full discretization of state and control variable profiles, for example using orthogonal collocation (Čižniar et al., 2005). The resulting model is a mixed-integer nonlinear programming (MINLP).

3. Application

In order to illustrate the procedural model design strategy, a system with competitive reactions is considered, where different products should be introduced in the plant production planning. The problem is solved through MLDO formulation, reformulation to MIDO and direct-simultaneous resolution approach. The obtained MINLP after the discretization is implemented in GAMS and solved with DICOPT 2x-C, using CONOPT 3.14 and CPLEX 12.2 to solve the NLP and MIP sub-problems. The process consists of the Denbigh System (Denbigh, 1958), with four competitive reactions (Eq. 2) to produce R, S, T and U. Kinetic data (Table 1) are adapted from Schweiger and Floudas (1999), defining 80°C as reference temperature.



Table 1: Kinetic constants ($r_i = c_i^n k_{0,i} \exp \frac{-E_{a,i}}{RT}$). Based on Schweiger and Floudas (1999).

| Reaction | $E_{a,i}$ [kcal/kmol] | $k_{0,i}$ [h^{-1}] or [$\text{m}^3/(\text{kmol}\cdot\text{h})$] | $k_{\text{reference},i}$ [h^{-1}] or [$\text{m}^3/(\text{kmol}\cdot\text{h})$] | N |
|----------|-----------------------|---|--|---|
| 1 | 1000 | 4.16 | 1 | 2 |
| 2 | 2580 | 23.75 | 0.6 | 1 |
| 3 | 1800 | 7.81 | 0.6 | 1 |
| 4 | 1210 | 0.56 | 0.1 | 2 |

As shown in Figure 2, the given process cell superstructure is composed by two reactors (U1, U2), the necessary splitters and mixers to provide flexibility to the process cell (S1, S2, M1, M2) and a separation unit to isolate the desired product from the mixture (D). Dynamic models are used for the reaction units, whereas an approximated linear model is employed in the separation unit. Different subsystems or configurations can be selected for the reactor network: a) one single reactor U1 or U2, b) both reactors U1 and U2 in series, or c) both reactors U1 and U2 in parallel.

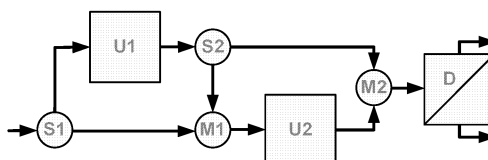


Figure 2: Superstructure of the process cell in the Case Study.

Due to a plant production expansion, components R, S, T and U are introduced in the market as new products. Hence, their procedural specification should be defined in the process cell, where building additional equipment is not considered. The production policy aims at minimizing the energy consumption. As a result, the design of all control recipes is obtained. In this stage, the energy consumption accounts principally for the required heat in the distillation unit to separate the final product. It is also considered to

be proportional to the amount of sub-products and un-reacted raw material. Then, the objective function z^{Energy} is calculated according to Eq. 3, where f is the relation between the waste and energy consumption, and X_p and $Batch_p$ are the conversion and the final amount of the desired product respectively. MLDO is used as control recipe optimization strategy, and obtained results are presented in Table 2. More details regarding operational decisions, namely profiles of actuation variables and stage transition times, are shown in Figure 3.

$$z^{Energy} = f \cdot Batch_p \cdot (1 - X_p) \quad (3)$$

Table 2: Optimal control recipes and resulting energy consumption to produce R, S, T and U according to an energy consumption minimization.

| Product | Batch Size [Kg] (fixed) | Resulting Control Recipe Parameters | | | Consumed energy [kWh/ batch] | |
|---------|-------------------------|-------------------------------------|---------------|---------------|------------------------------|---------------------------|
| | | Subsystem | T_{U1} [°C] | T_{U2} [°C] | | Processing time [h/batch] |
| R | 900 | U1, U2 parallel | 50 | 50 | 0.75 | 437 |
| S | 900 | U1, U2 series | 50 | 110 | 6.00 | 319 |
| T | 500 | U1, U2 series | 110 | 110 | 6.00 | 485 |
| U | 250 | U1, U2 series | 50 | 50 | 6.00 | 557 |

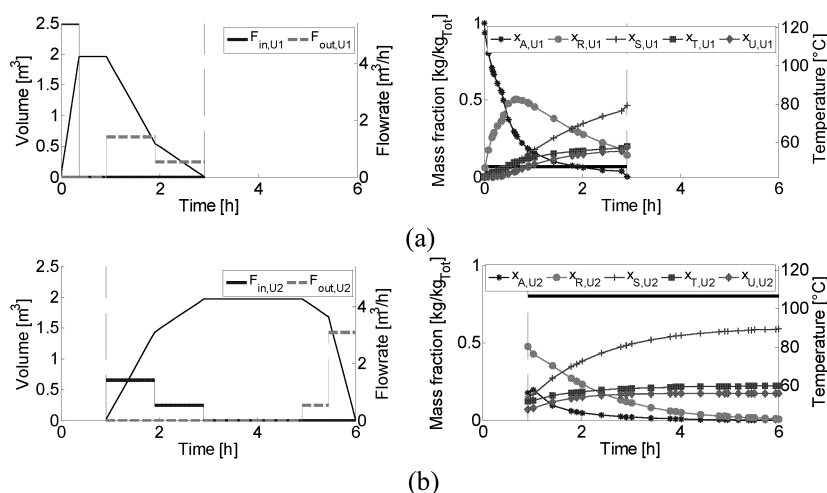


Figure 3: Reactors U1 (a) and U2 (b) working in series according to the optimal recipe for production of 1 batch of S. Actuation variables: flowrates and temperatures.

4. Conclusions

According to PSE actuation lines to face tight chemical production systems, some challenging directions have been addressed in this work. In particular, a problem which is multi-functional (i.e. process synthesis and optimal operation), multi-level (i.e. process cell and processing units) and based on global performance indicators (i.e. energy minimization) is successfully tackled. Systematic synthesis and optimization of

the procedural model has been newly undergone in a batch process framework to better exploit process adaptability. Promising model-based tools, such as GDP and discrete-continuous models, have been used to formulate the problem as a MLDO, an approach previously proposed by Oldenburg et al. (2003). Here, the MLDO approach has been extended to reactor network synthesis, rather than applied to isolated units. The extended approach is shown through a simple example that demonstrates its feasibility. In addition, the use of different configurations allows to achieve more suitable processing times and operating conditions, while reducing the energy consumption required for the same production performance. Further steps in this line will be focused on including multi-objective functions to evaluate the trade-offs between sustainability indicators and other driving forces such as other economic goals.

Acknowledgements

Financial support received from the Spanish Ministerio de Ciencia e Innovación and the European Regional Development Funds-ERDF (FPU grant and research project DPI2009-09386) is gratefully acknowledged.

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