An Effective MIDO Approach for the Simultaneous Cyclic Scheduling and Control of Polymer Grade Transition Operations

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In this work we propose a scheduling and control formulation for simultaneously addressing scheduling and control problems by explicitly incorporating process dynamics in the form of system constraints that ought to be met. The formulation takes into account the interactions between such problems and is able to cope with nonlinearities embedded into the processing system. The simultaneous scheduling and control problems is cast as a Mixed-Integer Dynamic Optimization (MIDO) problem where the simultaneous approach, based on orthogonal collocation on finite elements, is used to transform it into a Mixed-Integer Nonlinear Programming (MINLP) problem. The proposed simultaneous scheduling and control formulation is tested using a Methyl-Methacrylate CSTR where four different types of grades are manufactured. It is shown that the proposed methodology provides the best grade scheduling policy and optimal transition trajectories leading to maximum process profit.

1. Introduction

Traditionally, scheduling and control problems in chemical processes have been addressed in a separate way. From a scheduling point of view, the interest lies in determining optimal production sequences, production times for each product, switching times, leading to designs featuring maximum profit. Commonly, during this task, features related to the dynamic behavior of the underlying process are not taken into account. Similarly, when computing optimal transition trajectories (i.e. optimal values of the manipulated and controlled variables) between different set of products, one of the major objectives lies in determining the transition trajectory featuring minimum transition time. When addressing optimal control problems, it is normally assumed that the best production sequence has been determined in some way. Hence, normally scheduling features are neglected in optimal control formulations.

In this work we propose a simultaneous approach to address scheduling and control problems, particularly those emerging during grade transition operations in polymerization reactors. In the proposed formulation, integer variables are used to determine the best production sequence and continuous variables take into account production times, cycle time etc. Because, dynamic profiles of both manipulated and controlled variables are also decision variables, the resulting problem is cast as a Mixed-Integer Dynamic Optimization (MIDO) problem. To solve the MIDO problem we use a methodology which consists in transforming the MIDO problem into a MINLP that can be solved using standard methods such are the Outer-Approximation method. Roughly speaking, the strategy for solving the MIDO problem consists in using a simultaneous equation-oriented approach in which the optimal control problem is solved by transforming the set of ordinary differential equations into a set of algebraic equations. The simultaneous scheduling and control formulation is applied to a Methyl-Methacrylate CSTR where four different types of grades are manufactured.

2. Problem definition

Given are a number of products that are to be manufactured in a single continuous multiproduct CSTR. Steady-state operating conditions for manufacturing each product are also specified, as well as the demand rate and price of each product and the inventory and raw materials costs. The problem to be tackled consists in the simultaneous determination of the best production wheel (i.e. cyclic time and the sequence in which the products will be manufactured) as well as the transition times, production rates, length of processing times, amounts manufactured of each product, such that the profit is maximized subject to a set of scheduling and dynamic state constraints.

3. Scheduling and Control Formulation

In the following simultaneous scheduling and control (SSC) formulation, we assume that all products are manufactured in a single CSTR and that the products follow a production wheel meaning that all the required products are manufactured, in an optimal sequence to be determined, and that the sequence is repeated cyclically (see Pinto and Grossmann [1]).

- **Objective function.**

$$\max \quad \Bigg\{ \sum_{i=1}^{N_p} \frac{C_i^p W_i}{T_c} - \sum_{i=1}^{N_p} \frac{C_i^s (G_i - W_i)}{2\Theta_i T_c} - \sum_{k=1}^{N_s} \sum_{f=1}^{N_{fe}} h_{fk} \sum_{c=1}^{N_{cp}} \frac{C^r t_{fck} \Omega_{c,N_{cp}}}{T_c} \Big((x_{fck}^1 - \bar{x}_k^1)^2 + \ldots + (x_{fck}^n - \bar{x}_k^n)^2 + (u_{fck}^1 - \bar{u}_k^1)^2 + \ldots + (u_{fck}^m - \bar{u}_k^m)^2 \Big) \Bigg\} \tag{1}$$

1. Scheduling part.

$$\sum_{k=1}^{N_s} y_{ik} = 1, \ \forall i; \ \sum_{i=1}^{N_p} y_{ik} = 1, \ \forall k; \ y_{ik}^{'} = y_{i,k-1}, \ \forall i, k \neq 1; y_{i,1}^{'} = y_{i,N_s}, \ \forall i \tag{2}$$

$$W_i \geq D_i T_c, \ \forall i; \ W_i = G_i \Theta_i, \ \forall i; \ G_i = F^o(1 - X_i), \ \forall i \tag{3}$$

$$\theta_{ik} \leq \theta^{max} y_{ik},\ \forall i,k;\ \Theta_i = \sum_{k=1}^{N_s} \theta_{ik},\ \forall i;\ p_k = \sum_{i=1}^{N_p} \theta_{ik},\ \forall k \tag{4}$$

$$z_{ipk} \geq y'_{pk} + y_{ik} - 1,\ \forall i,p,k \tag{5}$$

$$\theta_k^t = \sum_{i=1}^{N_p} \sum_{p=1}^{N_p} t_{pi}^t z_{ipk},\ \forall k;\ t_1^s = 0; t_k^e = t_k^s + p_k + \sum_{i=1}^{N_p} \sum_{p=1}^{N_p} t_{pi}^t z_{ipk},\ \forall k \tag{6}$$

$$t_k^s = t_{k-1}^e,\ \forall k \neq 1;\ t_k^e \leq T_c,\ \forall k;\ t_{fck} = (f-1)\frac{\theta_k^t}{N_{fe}} + \frac{\theta_k^t}{N_{fe}} \gamma_c,\ \forall f,c,k \tag{7}$$

2. Dynamic Optimization part.

   To address the optimal control part, the so-called simultaneous approach [2] for solving dynamic optimization problems was used. In this approach the dynamic mathematical model representing system behavior is discretized using the method of orthogonal collocation on finite elements.

$$x_{fck}^n = x_{o,fk}^n + \theta_k^t h_{fk} \sum_{l=1}^{N_{cp}} \Omega_{lc} \dot{x}_{flk}^n,\ \forall n,f,c,k \tag{8}$$

$$x_{o,fk}^n = x_{o,f-1,k}^n + \theta_k^t h_{f-1,k} \sum_{l=1}^{N_{cp}} \Omega_{l,N_{cp}} \dot{x}_{f-1,l,k}^n,\ \forall n, f \geq 2, k \tag{9}$$

$$\dot{x}_{fck}^n = f^n(x_{fck}^1, \ldots, x_{fck}^n, u_{fck}^1, \ldots u_{fck}^m),\ \forall n,f,c,k \tag{10}$$

$$x_{in,k}^n = \sum_{i=1}^{N_p} x_{ss,i}^n y_{i,k},\ \forall n,k \tag{11}$$

$$\bar{x}_k^n = \sum_{i=1}^{N_p} x_{ss,i}^n y_{i,k+1},\ \forall n, k \neq N_s;\ \bar{x}_k^n = \sum_{i=1}^{N_p} x_{ss,i}^n y_{i,1},\ \forall n, k = N_s \tag{12}$$

$$u_{in,k}^m = \sum_{i=1}^{N_p} u_{ss,i}^m y_{i,k},\ \forall m,k;\ \bar{u}_k^m = \sum_{i=1}^{N_p} u_{ss,i}^m y_{i,k+1},\ \forall m, k \neq N_s - 1 \tag{13}$$

$$\bar{u}_k^m = \sum_{i=1}^{N_p} u_{ss,i}^m y_{i,1},\ \forall m, k = N_s \tag{14}$$

$$x_{N_{fe},N_{cp},k}^n = \bar{x}_k^n,\ \forall n,k;\ u_{1,1,k}^m = u_{in,k}^m,\ \forall m,k \tag{15}$$

$$u_{N_{fe},N_{cp},k}^m = \bar{u}_{in,k}^m,\ \forall m,k;\ x_{o,1,k}^n = x_{in,k}^n,\ \forall n,k \tag{16}$$

$$x_{min}^n \leq x_{fck}^n \leq x_{max}^n, \forall n,f,c,k;\ u_{min}^m \leq u_{fck}^m \leq u_{max}^m, \forall m,f,c,k \tag{17}$$

4. Application example

To analyze the simultaneous scheduling and control problem we consider grade transitions in a bulk free-radical isothermal Methyl-Methacrylate CSTR previously described by Congalidis et al. [3] and used by Mahadevan et al. [4] to address grade transition problems from a control point of view. The mathematical model was cast in dimensionless form by dividing each state and flow rates of monomer and initiator by their maximum expected values.

$$\frac{dx_1}{dt} = -\frac{V}{\hat{Q}_m}(k_p + k_{fm})x_1\sqrt{\frac{2f^* k_i \hat{C}_i x_2}{k_{td} + k_{tc}}} + \bar{Q}_m(x_{1_{in}} - x_1) \tag{18}$$

$$\frac{dx_2}{dt} = -\frac{V k_i}{\hat{Q}_m}x_2 + \frac{1}{\hat{Q}_m \hat{C}_i}(\hat{Q}_i \hat{C}_i x_{2_{in}} \bar{Q}_i - \bar{Q}_m \hat{Q}_m \hat{C}_i x_2) \tag{19}$$

$$\frac{dx_3}{dt} = \frac{V(0.5k_{tc} + k_{td})}{\hat{Q}_m \hat{D}_0}\left[\frac{2f^* k_i \hat{C}_i x_2}{k_{td} + k_{tc}}\right] + \frac{V k_{fm} \hat{C}_m}{\hat{Q}_m \hat{D}_0} x_1 \sqrt{\frac{2f^* k_i \hat{C}_i x_2}{k_{td} + k_{tc}}} - \bar{Q}_m x_3; \tag{20}$$

$$\frac{dx_4}{dt} = \frac{V M_m (k_p + k_{fm})\hat{C}_m}{\hat{Q}_m \hat{D}_1} x_1 \sqrt{\frac{2f^* k_i \hat{C}_i x_2}{k_{td} + k_{tc}}} - \bar{Q}_m x_4; \tag{21}$$

where $x_1 = \frac{C_m}{\hat{C}_m}, x_2 = \frac{C_i}{\hat{C}_i}, x_3 = \frac{D_0}{\hat{D}_0}, x_4 = \frac{D_1}{\hat{D}_1}, x_{1_{in}} = \frac{C_{m_{in}}}{\hat{C}_m}, x_{2_{in}} = \frac{C_{i_{in}}}{\hat{C}_i}, \bar{Q}_m = \frac{Q_m}{\hat{Q}_m}, \bar{Q}_i = \frac{Q_i}{\hat{Q}_i}$. In Table 1 information regarding steady-state design and reactor scaling is shown.

For testing our simultaneous scheduling and control formulation four polymer grades (A, B, C, D) were defined which correspond to molecular weight distributions of 15000, 25000, 35000 and 45000. The initiator flow rate (Q_i) was selected as the manipulated variable to achieve grade transition. Table 2 contains the steady-state values of the states and the manipulated variable leading to manufacture each one of the A, B, C and D grades. Also shown in Table 2 are the demand rate and cost of each grade.

The simultaneous scheduling and control formulation, as represented by Equations (1)-(17), was solved using GAMS/SBB, a MINLP solver embedded in GAMS which uses a branch and bound techniques for solving MINLP's. The problem size consisted of 2897 constraints, 3138 continuous variables and 96 integer variables. The problem was started solving first a relaxed version of the MINLP (4 s) and used to initialize the MINLP which was solved in 430 s cpu time. Table 3 shows the results of solving the scheduling and control problem. As can be seen, the optimizer selected the cyclic sequence $A \rightarrow D \rightarrow C \rightarrow B$ for the production wheel with a cycle time of 400 hrs. The formulation clearly assigns one of the larger processing times (100 h) to the more valuable grade D and the shortest processing time (80 h) to the less valuable grade A.

As a way to understand the role of process dynamics in the grade transition sequence that was selected, the MMA polymerization CSTR was linearized around each one of the steady-state design conditions shown in Table 2. In all the cases, the dominant eigenvalue was always -1, which is an indication that all the grades have similar open-loop constant times. This means that, the transitions are dominated by cost and are slightly influenced by process dynamics.

Table 1
Steady-state design and scaling information.

Q_m	1	Monomer feed stream [m3/h]
V	0.1	Reactor volume [m3]
$C_{i_{in}}$	8	Feedstream initiator concentration [kmol/m3]
M_m	100.12	Monomer molecular weight [kg/kmol]
$C_{m_{in}}$	6	Feedstream monomer concentration [kmol/m3]
f^*	0.58	Initiator efficiency
k_{tc}	1.3281x10^{10}	Termination by coupling rate constant [m3/(kmol-h)]
k_{td}	1.093x10^{11}	Termination by disproportionation rate constant [m3/(kmol-h)]
k_i	1.0255x10^{-1}	Initiation rate constant [1/h]
k_p	2.4952x10^6	Propagation rate constant [m3/(kmol-h)]
k_{fm}	2.4522x10^3	Chain transfer to monomer rate constant [m3/(kmol-h)]
$\hat{C}_m$	5.7768	Maximum value of monomer concentration [kmol/m3]
$\hat{C}_i$	0.41534	Maximum value of initiator concentration [kmol/m3]
$\hat{D}_0$	5.4794x10^{-3}	Maximum value of zeroth moment
$\hat{D}_1$	82.219	Maximum value of first moment
$\hat{Q}_i$	0.05245	Maximum value of initiator flow rate [m3/h]
$\hat{Q}_m$	1	Maximum value of monomer flow rate [m3/h]

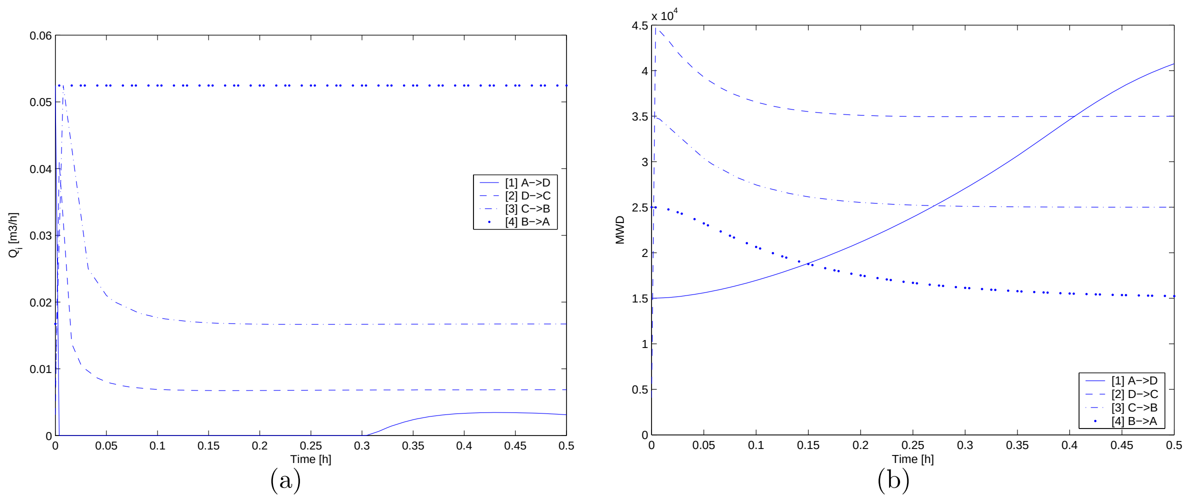

Figure 1. Dynamic behavior of the MMA polymerization system during grade transition. (a) The initiator flow rate (Q_i) is the manipulated variable, (b) The average molecular weight distribution (MWD) was one of the variables to be tracked during grade transition.

Table 2
Grade design information. The demand rate is in [kg/h] and the price in [$/kg].

Grade	Q_i	C_m	C_i	D_0	D_1	MWD	Demand rate	Price
A	0.05245	5.1788	0.4153	0.0055	82.2185	15000	0.8	10
B	0.01673	5.5068	0.1325	0.0020	49.3761	25000	0.7	12
C	0.006863	5.6745	0.0543	0.0009	32.5877	35000	1	13
D	0.003114	5.7768	0.0247	0.0005	22.3467	45000	0.8	15

Table 3
Simultaneous scheduling and control results for grade transtion in a MMA polymerization CSTR. The objective function value is $ 54 and 400 h of total cycle time.

Slot	Product	Process time [h]	Production rate [Kg/h]	w [Kg]	Transition Time [h]	T start [h]	T end [h]
1	A	80	4	320	5	0	85
2	D	100	5	500	5	85	190
3	C	100	4	400	10	190	300
4	B	95	5	475	5	300	400

5. Conclusions

In this work we addressed the simultaneous scheduling and control problem for grade transition in a MMA polymerization CSTR. Rather than assuming constant transition times and neglecting process dynamics, a mathematical model, able to describe dynamic process behavior during product transition, was embedded into the optimization formulation. Solving the scheduling and control problem taking into account process dynamics is the rigorous way to address scheduling problems. There is always a risk of getting suboptimal solutions when process dynamics are neglected.

REFERENCES

1. J.M. Pinto and I.E. Grossmann, Computers.Chem.Engng. 18 (1994) 797.
2. Kameswaran, S. and Lorenz T. Biegler, “Simultaneous Dynamic Optimization Strategies: Recent Advances and Challenges,” Proceedings of CPC7, accepted for publication (2005)
3. J.P. Congalidis, J.R. Richards and W.H. Ray, AICHE J, 35 (1989) 891.
4. R. Mahadevan, F. Doyle, A.C. Allcock, AICHE J, 48 (2002) 1754.