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Integrated Production Scheduling and Model Predictive Control of Continuous Processes

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The integration of production management and process control decisions is critical for improving economic performance of the chemical supply chain. A novel framework for integrating production scheduling and model predictive control (MPC) for continuous processes is proposed. Our framework is predicated on using a low-dimensional time scale-bridging model (SBM) that captures the closed-loop process dynamics over the longer time scales that are relevant to scheduling calculations. The SBM is used as a constraint in a mixed-integer dynamic formulation of the scheduling problem. To synchronize the scheduling and MPC calculations, a novel scheduling-oriented MPC concept is proposed, whereby the SBM is incorporated in the expression of the controller as a (soft) dynamic constraint and allows for obtaining an explicit description of the closed-loop process dynamics. Our framework scales favorably with system size and provides desirable closed-loop stability and performance properties for the resulting integrated scheduling and control problem. *AIChE J*, 61: 4179–4190, 2015
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Introduction

The process industry is in a permanent quest to improve economic and environmental performance. Enterprise-wide optimization[1] and smart manufacturing,[2–4] which promote sharing information and improving decisions at all levels of the process control and operations hierarchy (Figure 1) have been identified as key directions to this end.

Under this impetus, progress has been made in achieving a tighter integration of the production management layers (planning and scheduling) of the hierarchy.[6] Similarly, the incorporation of economic considerations in the formulation of the supervisory control problem has received significant attention, giving rise to the economic model predictive control (EMPC) concept.[7–9]

In the same context, a strong connection between scheduling and supervisory control decisions represents a pivotal point in streamlining decision-making across the entire chemical supply chain. However, the integration of scheduling and control has received comparatively little attention in the past.[10] On the one hand, this is due to human factors: production scheduling and process control are typically the responsibility of separate entities in a commercial organization, and are carried out by personnel with different backgrounds and charged with different explicit objectives (e.g., increasing profit vs. ensuring stable and safe day-to-day operations).[11–13] On the other hand, several open technical problems must be resolved in order to fully integrate scheduling and control. These include, (1) dealing with the large-scale, stiff models required to account for the multiple time horizons of the two activities—days or weeks (for scheduling), seconds or minutes (for control), (2) ensuring closed-loop stability for the process under consideration, and (3) the closely-related issue of managing the real-time completion of the mixed-integer optimization calculations associated with the integrated problem.

Thus far, research on these challenges has followed two main paradigms[10]:

- *top-down* approaches focus on integrating information concerning process dynamics in a scheduling skeleton. Incorporating the full dynamic model of a large-scale process in a scheduling calculation with a relatively long time horizon is computationally expensive,[14,15] and both simultaneous[16–20] and sequential methods[14,21–23] have been proposed to solve this problem. Decomposition strategies[14,24–26] have also been developed to facilitate obtaining the solution in a reasonable amount of time.
- *bottom-up* approaches[7,27,28] focus on embedding economic considerations in the formulation of the control problem, and have, as mentioned, given rise to the EMPC formalism. Until now, however, conceptual studies and applications of EMPC to processes and energy systems where scheduling decisions would otherwise be highly relevant (e.g., electrolytic processing, power generation, refrigeration, and air conditioning[29–35]), have largely considered only continuous state and

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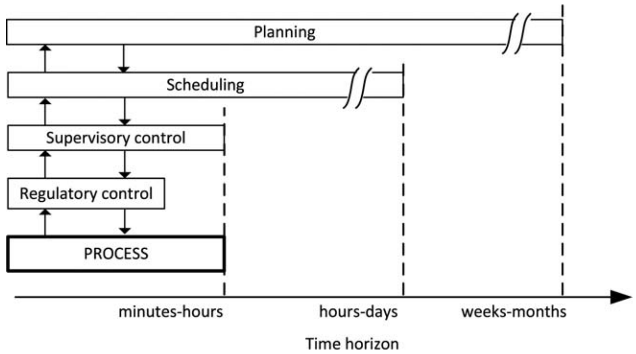

Figure 1. Decision-making hierarchy in process control and operations. Adapted from Ref. 5.

decision variables. Thus, while the underpinnings of EMPC are well-suited to dealing with combined scheduling and control decisions, incorporating binary decision variables and using scheduling-length prediction horizons remain open issues[36] that must be addressed before EMPC can be used in the integration of scheduling and control.

In this article, we describe a novel framework for integrating production scheduling and process control for continuous processes, focusing in particular on model-predictive control (MPC) as the most prevalent control approach in the chemical industry.[37] Our framework is predicated on:

1. developing a low-dimensional model of the dynamics of the process and the supervisory MPC controller, which we will refer to as the time scale-bridging model (SBM).[38] The SBM captures the closed-loop input-output behavior of the process and the MPC controller, describing the evolution in time of the scheduling-relevant process quality variables as a function of the controller setpoints.

2. using the low-order SBM as a constraint in the scheduling calculations. The scheduling problem is a mixed-integer dynamic optimization (MIDO), in which both production management and process dynamics are accounted for. The solution of this MIDO comprises a time-varying, step-wise setpoint signal.

3. tracking the setpoint signal in closed loop using the MPC controller described above, which results in imposing the optimal production sequence and optimal transition trajectory between products, and ensures robustness to plant-model mismatch and disturbances.

The key elements of our approach are summarized in Figure 2.

To overcome the inherent difficulty of obtaining closed-form expressions for MPC controllers, we propose a novel scheduling-oriented MPC formulation in which the SBM is incorporated as a (soft) dynamic constraint, thereby imposing the desired closed-loop behavior of the process.

The article is organized as follows: we proceed with the mathematical description of the process systems under consideration and define the scheduling and control problems. We then introduce time scale-bridging models, followed by describing the reformulated low-order scheduling MIDO and scheduling-oriented MPC. We subsequently review numerical implementation and solution strategies for the proposed integrated scheduling and control framework. The article concludes with an illustrative case study and a discussion of the theoretical developments and simulation results.

Problem Formulation

System description

In this work, we deal with continuous process systems, which we assume to be modeled in the state-space form

$$\dot{\mathbf{x}}=\mathbf{f}(\mathbf{x})+\mathbf{G}(\mathbf{x})\mathbf{u} \tag{1a}$$

$$\mathbf{y}=\mathbf{h}(\mathbf{x}) \tag{1b}$$

where $\mathbf{x} \in D_x \subset \mathbb{R}^{n_x}$ are the state variables, $\mathbf{u} \in D_u \subset \mathbb{R}^{n_u}$ are manipulated inputs, $\mathbf{f} : D_x \to D_x$ and $\mathbf{G}$ is a $n_x \times n_u$ dimensional function with every column $\mathbf{g} : D_x \to D_x$. $\mathbf{y} \in D_y \subset \mathbb{R}^{n_y}$ are the process outputs (quality variables) and $\mathbf{h} : D_x \to D_y$. Based on the values of $\mathbf{y}$, we can define $i=1, \ldots, N_p$ products, each having distinct quality $\mathbf{y}_i$. We assume that a unique set of inputs $\mathbf{u}_i$ corresponds to each product $\mathbf{y}_i$ (i.e., no input or output multiplicity) and the state space D_x is such that each product $\mathbf{y}_i$ can be reached from at least one other product $\mathbf{y}_{i'}$ via a connected path.

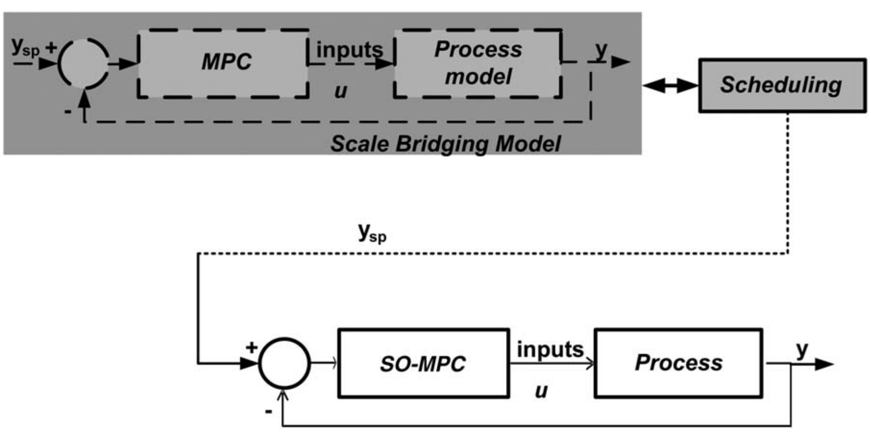

Figure 2. Elements of the proposed SBM-based integrated scheduling and control formulation: the scheduling mechanism produces a step-wise setpoint signal $y^l_{sp}(t)$ for each quality variable y^l, which reflects the optimal sequencing of products and production times, accounting for the transition time between products.

This signal is tracked by the scheduling-oriented MPC (SO-MPC), which results in imposing the optimal production sequence and optimal transition trajectory between products, and ensures robustness to plant-model mismatch and disturbances. Also see Du et al.[38]

We assume that the following properties are known for each product i: inventory cost $c_{\text{storage},i}$, sales price π_i, and demand rate $\delta_{r,i}$ (or absolute demand δ_i).

Production scheduling

The production scheduling problem is formulated (Flores-Tlacuahuac and Grossmann,[16] see also Du et al.[38]) in terms of identifying the optimal production sequence (order in which products i are made), product quantities ω_i as well as the production time for each product, which maximize operational profit per unit time

$$J_{\text{scheduling}} = \frac{1}{T_c}\left(\Gamma_p - \Gamma_s\right) \tag{2}$$

where Γ_p represents the profit from product sales and Γ_s is the cost of product storage.

$$\Gamma_p = \sum_{i=1}^{N_p} \pi_i \omega_i \tag{3}$$

$$\Gamma_s = \sum_{i=1}^{N_p}\sum_{s=1}^{N_s} \omega_{i,s} c_{\text{storage},i}\left(T_c - t_s^f\right) \tag{4}$$

We use a slot-based, continuous-time scheduling formulation, whereby the assignment of products to the N_s time slots is done via binary variables $z_{i,s}$. We assume that only one product is made in each time slot

$$\sum_{i=1}^{N_p} z_{i,s} = 1 \;\forall s \tag{5a}$$

We assume that production is cyclical, and—for simplicity—that a product i can only be made once in each production cycle

$$\sum_{s=1}^{N_s} z_{i,s} = 1 \;\forall i \tag{5b}$$

The number of time slots is assumed to be equal to the number of products

$$N_p = N_s \tag{5c}$$

The timing of each slot s is defined based on the start and end times, respectively, t_s^s and t_s^f, the production time t_s^p, and the transition time τ_s, which accounts for the time required to switch from producing product i' in slot $s-1$ to making product i in slot s

$$\begin{aligned} t_s^f &= t_s^s + \tau_s + \sum_{i=1}^{N_p} t_{i,s}^p \quad \forall s \\ t_{i,s}^p &\le z_{i,s} t_s^{p^{\max}} \quad \forall i, \forall s \end{aligned} \tag{5d}$$

The start time of each slot coincides with the end time of the previous slot

$$t_s^s = t_{s-1}^f \quad \forall s \ne 1 \tag{5e}$$

and the makespan corresponds to the end time of the last slot

$$t_s^f = T_c \;\; s = N_s \tag{5f}$$

Additional constraints are related to demand satisfaction. These can be expressed in terms of known demand rates $\delta_{r,i}$ as discussed in Flores-Tlacuahuac and Grossmann[16]

$$\begin{aligned} \omega_i &\ge \delta_{r,i} T_c \quad \forall i \\ \omega_i &\le \lambda_{r,i}\delta_{r,i} T_c \;\; \forall i \end{aligned} \tag{5g}$$

where the amounts of product manufactured are calculated from

$$\begin{aligned} \omega_{i,s} &= q_i t_{i,s}^p \quad \forall i, \forall s \\ \omega_i &= \sum_{i=1}^{N_s} \omega_{i,s} \;\; \forall i \end{aligned} \tag{5h}$$

Remark 1. *In the case of noncyclical production, an absolute demand δ_i can be specified for each product i, in which case the constraint (5g) becomes*

$$\begin{aligned} \omega_i &\ge \delta_i \;\; \forall i \\ \omega_i &\le \lambda_i \delta_i \;\; \forall i \end{aligned} \tag{5g$'$}$$

Formulating the problem in terms of absolute product demand is complementary but not equivalent to the formulation based on demand rate. Given a demand value, the corresponding demand rate cannot be immediately determined owing to the fact that the cycle time T_c is not known ahead of time. Likewise, if the demand rate is known, corresponding fixed demand values cannot be calculated since T_c is not known a priori. Nevertheless, assuming that one problem is solved, the corresponding problem can be formulated as well. For example, absolute demand can be defined in terms the (specified) product demand rate and the (optimal) cycle time, $\delta_i = \delta_{r,i} T_c$ (and viceversa).

Remark 2. *The constants $\lambda_{r,i}$ (and, respectively, λ_i) help define the upper bounds on the production and, respectively, production rate of product i. Choosing values slightly above unity will prevent overproduction, potentially at the cost of obtaining lower values of the objective function $J_{scheduling}$ in (2) than in the case when no upper bound is imposed. Nevertheless, choosing tight upper bounds is an important practical consideration given limitations in storage capacity, in the processing capacity of a process downstream or in the absorbtion capacity of the market.*

Dynamic considerations and integrated scheduling and control

The objective function (2) and the constraints (5) fully define the scheduling problem, with the exception of the transition times τ_s, which depend on the process dynamics and the performance of the control system. One possibility for identifying these transition times (in addition to creating static "transition tables" based on exhaustive testing) is the incorporation of the dynamic process model (1) as an additional set of constraints. This gives rise to a large-scale problem (note that further constraints involving the process input and/or states can be easily incorporated)

$$\begin{aligned} &\max_{\mathbf{u},\mathbf{z},t_s^p,t_s^s,t_s^f,\tau_s,\omega_i,T_c} J_{\text{scheduling}} \\ &\text{s.t. scheduling constraints (5)} \\ &\text{dynamic process model (1)} \\ &\mathbf{x},\mathbf{y},\mathbf{u} \in D_{\mathbf{x},\mathbf{y},\mathbf{u}} \end{aligned} \tag{6}$$

We will refer to this formulation of the integrated scheduling and control problem as "Problem P1." We note that the solution of P1 provides not only the production sequencing and timing information (given by the optimal values of $\mathbf{z}, t_s^p, t_s^s, t_s^f, \tau_s, \omega_i, T_c$), but also the manipulated input signal $\mathbf{u}(t)$ that imposes the optimal production sequence on the dynamical system. This highlights one of the drawbacks of this monolithic approach: from a control perspective, $\mathbf{u}(t)$ represents an open-loop control solution, which is susceptible to performance degradation and even loss of stability if the model (1) is not perfect (i.e., in the presence of plant-model mismatch) or in the face of disturbances. Furthermore, the solution of this problem is computationally expensive, especially when the dimension of the state space $\mathbb{R}^{n_x}$ of the dynamic model (1) is large,[14,15] in which case model reduction techniques (e.g., Hahn and Edgar[39]; Baldea and Daoutidis[40]) combined with advanced numerical solution approaches[18] should be considered.

The above observations provide the incentive for (1) reducing the dimension of the integrated scheduling/control problem and, (2) devising a closed-loop implementation strategy that ensures operational performance in the presence of disturbances and/or plant-model mismatch.

Integrated Scheduling and MPC Using Time Scale-Bridging Models

Time scale-bridging

In our previous work,[38,41] we introduced the concept of time scale-bridging model (SBM), as a representation of the closed-loop input-output behavior of the process and its control system. Thus, the SBM captures the dynamics between the controller setpoints $\mathbf{y}_{\text{sp},i}$ corresponding to products i, and the process output $\mathbf{y}$. The role of the control system is then to eliminate the offset $\mathbf{y}_{\text{sp},i}-\mathbf{y}$ in each production slot, so that the desired product is manufactured at the correct specification.

We represent the control law in the general form

$$0=\kappa(\dot{\mathbf{x}}, \mathbf{x}, \dot{\mathbf{y}}, \mathbf{y}, \mathbf{y}_{\text{sp}}, \mathbf{u}, \beta) \tag{7}$$

and assume that it imposes a closed-loop behavior that can be explicitly characterized by an expression of the form

$$\frac{d\mathbf{y}}{dt}=\Psi(\mathbf{y}, \mathbf{y}_{\text{sp}}, \beta) \tag{8}$$

which then constitutes the SBM (where β are tunable controller parameters).

With this expression, the integrated scheduling and control problem takes the form

$$\begin{aligned} \max_{\mathbf{u},\mathbf{z},t_s^p,t_s^s,t_s^f,\tau_s,\omega_i,T_c} \quad & J_{\text{scheduling}} \\ \text{s.t.} \quad & \text{scheduling constraints } (5) \\ & \text{scale-bridging model } (8) \\ & \mathbf{y} \in D_{\mathbf{y}} \end{aligned} \tag{9}$$

Equation 9, in tandem with the control law (7) represents an integrated scheduling and control mechanism, which we will refer to as "Problem P2." The scheduling component (9) is aware of the (closed-loop) process dynamics via the SBM constraint. The scheduling calculation provides the time-varying setpoint to be implemented by the control system (7) in order to impose the optimal production sequence and optimal transition trajectory between products.

Remark 3. *We note that in practice the number of process quality variables that are of interest to scheduling is likely much lower than the number of process states (i.e., the dimension of the output vector* $\mathbf{y}$ *is much lower than the dimension of the state vector* $\mathbf{x}$*, i.e.,* $n_y \ll n_x$*). As the SBM captures the dynamics of the system outputs, its dimension is dictated by the dimension of* $\mathbf{y}$ *and will thus be much lower than the size of the dynamic model (1). Consequently, the dimension of the dynamic model in the MIDO (9) is lower than that in the monolithic formulation P1, which makes P2 less computationally expensive.*

Another significant benefit of the proposed integrated scheduling and control formulation is that the scheduling solution is implemented in closed-loop, thereby ensuring performance in the presence of disturbances or modeling errors.

Remark 4. *The use of SBMs to represent the process dynamics in scheduling calculations is well motivated by previous process systems research (e.g., works by Kumar and Daoutidis[42]; Contou-Carrère et al.[43]; Jogwar et al.[44]; Baldea and Daoutidis[40]; Baldea et al.[45]). These studies have revealed that the dynamic behavior of process quality variables (e.g., product purity, total material inventory, and production rate) over time scales that are relevant to scheduling can be described by low-order models whose dimensions are comparable with the number of chemical compounds present in the process.*

Remark 5. *Several researchers (e.g., Wan et al.[46]; Sung and Maravelias[47,48]) have focused on identifying "surrogate," low-order models for the solution of operational problems. The SBM-based approach introduced in this article can in a sense be regarded as an extension of these efforts (which used static low-order representations) to the dynamic realm, a necessary feature for addressing the integration of scheduling and process control.*

Evidently, deriving an expression for the SBM is a central challenge. In our previous work,[38,41] we have shown that a linear SBM of the form

$$\sum_{m=0}^{r^l} \beta_{l,m} \frac{d^m y^l}{dt^m} = y^l_{\text{sp}} \tag{10}$$

where r^l is the relative degree* and $\beta_{l,m}$ are elements of the set of tuning parameters β, can be imposed using an input-output linearizing supervisory controller with integral action as described by Daoutidis and Kravaris.[49] However, input-output linearization is typically applicable to "square" systems, having an equal number of inputs and outputs[52] and, furthermore, cannot explicitly account for constraints on the process states $\mathbf{x}$ and inputs $\mathbf{u}$.

In this article, we work on problem P2, but consider the case when the controller used to impose a closed-loop input-output process behavior of the form (10) is of the model-predictive type. Our work is motivated by the fact that many practical systems are neither square nor unconstrained, and model predictive control (MPC) is recognized precisely for its

*The relative degree, or relative order, characterizes how "directly" a system output is affected by an input variable.[49] For a single-input, single-output system of the form

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{f}(\mathbf{x})+\mathbf{g}(\mathbf{x})u \\ y &= \mathbf{h}(\mathbf{x}) \end{aligned}$$

the relative degree is defined[50] as the value r, such that

- $L_{\mathbf{g}}L_{\mathbf{f}}^k\mathbf{h}(\mathbf{x})=0, \quad \forall k < r-1$
- $L_{\mathbf{g}}L_{\mathbf{f}}^{r-1}\mathbf{h}(\mathbf{x}) \neq 0$

where $L_{\mathbf{g}}\mathbf{h}$ represents the Lie (directional) derivative of function $\mathbf{h}$ along function $\mathbf{g}$. This definition can be extended to multivariate systems (see e.g., the classic book by Isidori,[50] p. 235). The relative degree can be determined by successively computing the relevant Lie derivatives until the above conditions are met. Alternatively, a graph-theoretical approach is available as described in Daoutidis and Kravaris.[51]

ability of handling input, state and output constraints, and non-square systems. In what follows, we define a special scheduling-oriented MPC formulation, which will support our efforts in the sequel.

Scheduling-Oriented MPC

The MPC control law can be written in the general form[53]

$$\begin{aligned} &\min_{\mathbf{u}} J_{\text{control}} = \int_{t_0}^{t_0+T_P} \|\mathbf{u}\|_{\mathbf{R}} + \|\mathbf{y}_{\text{sp}} - \mathbf{y}(t)\|_{\mathbf{Q}} dt \\ &\text{s.t. process model (1)} \\ &\mathbf{x}, \mathbf{y}, \mathbf{u} \in D_{\mathbf{x},\mathbf{y},\mathbf{u}} \end{aligned} \tag{11}$$

where $\|\mathbf{a}\|_{\mathbf{S}} = \mathbf{a}^T\mathbf{S}\mathbf{a}$, and matrices $\mathbf{R}$ and $\mathbf{Q}$ are symmetric and, respectively, positive semidefinite and positive definite. T_P is the prediction horizon.

In this article, we focus on the above implicit (in the sense that the control law is not available in closed-form) MPC formulation as the control companion to P2. This formulation has gained popularity in industry over the past decades[37] but presents the major challenge of precluding the derivation of an explicit expression of the closed-loop dynamics (i.e., the desired SBM).[†]

To overcome this challenge, we propose reformulating the MPC problem (11) to impose a prespecified input-output behavior. To this end, we replace the tracking component of the MPC objective function J_{control} in (11) with a dynamic tracking constraint of the form (10), which represents precisely the SBM that we are searching. Thus, we obtain the scheduling-oriented MPC formulation

$$\begin{aligned} &\min_{\mathbf{u}} \bar{J}_{\text{control}} = \int_{t_0}^{t_0+T_P} \|\mathbf{u}\|_{\mathbf{R}} dt \\ &\text{s.t. process model (1)} \\ &\quad \text{scale-bridging model} \sum_{m=0}^{r^l} \beta_{l,m} \frac{d^m y^l}{dt^m} = y^l_{\text{sp}} \\ &\quad \mathbf{x}, \mathbf{y}, \mathbf{u} \in D_{\mathbf{x},\mathbf{y},\mathbf{u}} \end{aligned} \tag{12}$$

which, in conjunction with the scheduling component (Problem P2), which provides the setpoint sequence $\mathbf{y}_{\text{sp}}$, constitutes an integrated production scheduling and model predictive framework for continuous process systems of the form (1). A block diagram of the proposed integrated scheduling and MPC approach is shown in Figure 2, emphasizing the fact that in this scheme the process is permanently operating *in closed loop*.

Remark 6. *For feasibility reasons, the SBM constraint in (12) should be implemented as a soft constraint. The feasibility of (12) is also influenced by the tuning parameters $\beta_{l,m}$, which should be chosen in accordance with the process dynamics and the corresponding time constants; more specifically, an overly aggressive choice of the closed-loop time constants $\beta_{l,m}$ may make it difficult to satisfy the SBM constraint, while a conservative set of values will not cause SBM infeasibility but may lead to an overly conservative scheduling solution. These issues are discussed more extensively in the case study presented in the article.*

[†]We note that an explicit formulation of the MPC controller can be derived in parametric form,[54] and has been recently used to explore integrated scheduling and control approaches for process systems.[55,56]

Remark 7. *The MPC formulation in (12) lends itself naturally to an interpretation from the economic MPC (EMPC) point of view, whereby the weights* $\mathbf{R}$ *of the inputs* $\mathbf{u}$ *can be meaningfully chosen as the actual prices of the manipulated inputs of the system.*

Remark 8. *The use of dynamic constraints of the type of the SBM proposed above has been described earlier by Young et al.[57] in the context of improving tracking performance for an industrial nonlinear MPC controller, however, without incorporating scheduling considerations in the problem formulation. More recently, Wallace et al.[58] have reported using additional first-order linear dynamic constraints to shape the closed-loop behavior of a heat pump operating under linear MPC, again without a scheduling-specific focus. In a different vein, Soroush and Kravaris[59] have shown that, under specific conditions, a linear reference trajectory obtained by filtering the setpoint can be tracked exactly with an MPC controller, thereby providing a well-defined closed-loop input-output behavior.*

Remark 9. *From a broader perspective, we note that several literature contributions attempt to define closed-loop performance in terms of tracking a prescribed trajectory with a well defined accuracy. These include, for example, performance "funnels",[60] and the grade transition framework reported in Flores-Tlacuahuac et al.[61] While these are similar in spirit to the proposed scheduling-oriented MPC, they do not consider the scheduling component that optimally orchestrates the transitions between the system states that correspond to different products.*

Implementation and Numerical Solution

Mixed-integer dynamic optimization (MIDO)

Both Problems P1 and P2 are MIDO problems. To obtain their solution, we use a simultaneous approach, which consists of converting the MIDO into a large scale mixed-integer nonlinear program (MINLP) using collocation on finite elements.[62]

In particular, we consider that each time slot consists of a transition period of length τ_s and a production period of length t^p_s, and impose that the product reaches the desired values of the quality variables y^l_{ss} at the end of the transition period.[16] Equivalently, the system reaches steady state at the end of the transition period, and remains at steady state during the production period. This allows us to consider system dynamics only during the transition period, and leave a single continuous decision variable (t^p_s, the length of production time) for the steady-state portion of each production time slot s.

For each transition period, we discretize the dynamic equations using a Radau quadrature.[63] Thus, for any state $x^l \in \mathbf{x}$ at collocation point j in finite element k in slot s (note that this discussion applies identically to variables $\mathbf{y}$ in Problem P2), we have[16]

$$x^l_{j,k,s} = x^l_{0,k,s} + \frac{\tau_s}{N_e} \sum_{m=1}^{N_{\text{cp}}} W_{m,j} \dot{x}^l_{m,k,s} \quad \forall x^l \in \mathbf{x};\ \forall k, s \tag{13a}$$

where W is the matrix of Radau quadrature weights, N_e is the number of finite elements for each transition period, such that the length of each finite element is $1/N_e$, and N_{cp} is the number of collocation points in each element. Furthermore, we impose state continuity by equating the value of the state at the beginning of each finite element with the value of the state at the last collocation point in the previous element.[16]

Table 1. Process Parameters for Exothermic CSTR[16]

Parameter	Values	Parameter Significance
N	5	E_a/RJc_f
J	100	$-\Delta H/\rho C_p$
α	0.000195	Dimensionless heat-transfer area
k_{10}	300	Pre-exponential factor
T_{feed}	300	Feed temperature
c_f	7.6	Feed concentration
$T_{coolant}$	290	Coolant temperature

$$x^l_{0,k,s}=x^l_{0,k-1,s}+\frac{\tau_s}{N_e}\sum_{m=1}^{N_{cp}} W_{m,N_{cp}}\dot{x}^l_{m,k-1,s} \quad \forall x^l \in \mathbf{x}; \forall k>1; \forall s \tag{13b}$$

Per our previous assumption, the value of $x^l_{0,1,s}$ of the state in the first finite element should be the same as its steady-state value in the previous time slot[16]

$$x^l_{0,1,s}=\sum_{i=1}^{N_p} z_{i,s-1}x^l_{ss,i} \quad \forall x^l \in \mathbf{x}; \forall s \tag{13c}$$

Moreover, x^l should be close to its steady-state value at the end of the transition period[16]

$$\begin{aligned} x^l_{j,k,s} &\le (1+\varepsilon^l)\sum_{i=1}^{N_p} z_{i,s}x^l_{ss,i} \quad \forall j \ge \bar{j}, \forall k, \forall s \\ x^l_{j,k,s} &\ge (1-\varepsilon^l)\sum_{i=1}^{N_p} z_{i,s}x^l_{ss,i} \quad \forall j \ge \bar{j}, \forall k, \forall s \end{aligned} \tag{13d}$$

with $\bar{j}$ typically chosen to be close to the number of finite elements N_e and $\varepsilon^l>0$ is a small number.

Likewise, u^l should be at its steady-state value at the end of the transition period[16]

$$u^l_{N_{cp},N_e,s}=\sum_{i=1}^{N_p} z_{i,s}u^l_{ss,i} \quad \forall u^l \in \mathbf{u}; \forall s \tag{13e}$$

where $x^l_{ss,i} \in \mathbf{x}$ and $u^l_{ss,i}$ are the steady-state values of the state variables x^l and, respectively, input variables u^l, which correspond to the desired values of the quality variables $\mathbf{y}_i$ of product i.

The discretization (13) only ensures the continuity of the state variables $\mathbf{x}$ (respectively, of the quality variables $\mathbf{y}$ for Problem P2) and does not provide for any continuity properties for the input variables $\mathbf{u}$ (in P1). As a consequence, at some time instants the rate of change of $\mathbf{u}(t)$ could become very large. To address this issue, additional smoothness constraints of the form

$$|u^l_{j,k,s}-u^l_{j-1,k,s}| \le \rho^l_1 \quad \forall u^l \in \mathbf{u}; \forall j>1; \forall k; \forall s \tag{14a}$$

and

$$|u^l_{j,k,s}-u^l_{j,k-1,s}| \le \rho^l_2 \quad \forall u^l \in \mathbf{u}; \forall j; \forall k>1; \forall s \tag{14b}$$

are imposed (note that the weights ρ^l_1 and ρ^l_2 can be different for each input $u^l \in \mathbf{u}$). These weights can be defined in terms of rate-of-change restrictions on the manipulated inputs (a point that will be illustrated in the case study presented later in the article) and are similar to the penalty imposed on the rate of change of input variables in the "delta U" formulation of MPC.[5]

Then, the elements y^l_{sp} of the setpoint sequence $\mathbf{y}_{sp}$ to be imposed by the MPC are constructed from the solution of P2, as the stepwise signal

$$\begin{aligned} y^l_{sp}(t) &= \sum_{i=1}^{N_p} z_{i,s}y^l_{i,ss}\Big|\, t \in [t^s_s,\ t^f_s) \quad s=1,\ldots,N_s \\ y^l_{sp}(T_c) &= \sum_{i=1}^{N_p} z_{i,N_s}y^l_{i,ss} \end{aligned} \tag{15}$$

Remark 10. *In addition to providing a meaningful link between integrated scheduling and control, and a closed-loop implementation using MPC, the smoothness constraints (14) facilitate the direct (rather than iterative) computation of the optimal transition times between products. A further discussion on the iterative selection of transition times is available elsewhere.*[16,17]

MPC formulation

The feasibility of the scheduling-oriented MPC controller (12) is dependent on the choice of tuning parameters β selected for the SBM. As noted in Remark 6, the optimization problem (12) may become infeasible if the desired closed loop time constant (dictated by the selection of the values β) is much lower than the open-loop time constant of the system.

A feasible value of the closed-loop time constant (and, consequently, for β) can be obtained from the optimal values of the transition times τ_s, which are decision variables in the formulation (13) of the full-order Problem P1. Thus, a feasible (but likely conservative, upper bound) value for the closed loop time constant could be computed as $\max(\tau_s)$. Alternatively, the time constant could be estimated from an average of the values τ_s, in which case, as mentioned above, the problem (12) may become infeasible for some transitions.

This challenge can be addressed by reformulating the SBM dynamic constraint in (12) as a soft constraint. We will discuss this idea in more detail in the case study presented below; for more details regarding the use of soft constraints in MPC, the reader is referred to the works by Scokaert and Rawlings[64] and Kerrigan and Maciejowski.[65]

Illustrative Example

Problem description

We consider an exothermic multiproduct continuously stirred tank reactor adapted from Flores-Tlacuahuac and Grossmann.[16] The material and energy balance equations for the system are

Table 2. Process Conditions and Product Quality Variables for the CSTR (Adapted from Ref. 16)

Product i	$\delta_{r,i}$ (m^3/h)	q_i (m^3/h)	π_i ($\$/m^3$)	$c_{storage,i}$ ($\$/m^3/h$)	c_{ss}	T_{ss}	θ_{ss} (h)	$F_{c,ss}$ (m^3/h)
A	0.1318	1.1	180	5.0	0.0944	0.7766	20	340
B	0.2636	1.1	110	0.5	0.1367	0.7293	20	390
C	0.2636	1.1	60	2.2	0.1926	0.6881	20	430
D	0.1977	1.1	140	1.05	0.2632	0.6519	20	455

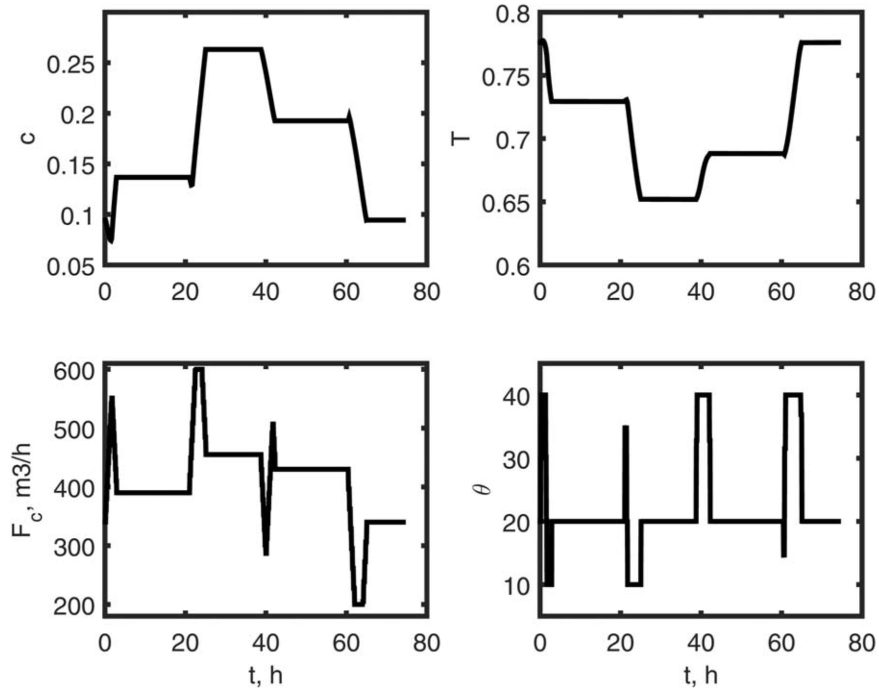

Figure 3. The evolution of the quality variables and process inputs for the optimal production sequence calculated based on the integrated scheduling and control formulation using the full process model (Problem P1).

$$\frac{dc}{dt} = \frac{1-c}{\theta} - k_{10} e^{-N/T} c \tag{16a}$$

$$\frac{dT}{dt} = \frac{T_f - T}{\theta} + k_{10} e^{-N/T} c - \alpha F_c (T - T_c) \tag{16b}$$

where c is the dimensionless concentration C/c_f, T is the dimensionless temperature, θ represents reactor residence time, k_{10} is the pre-exponential factor, and N is the activation energy. T_f denotes the dimensionless feed temperature (T_{feed}/Jc_f), T_c is the dimensionless coolant temperature $(T_{\text{coolant}}/Jc_f)$, α is the dimensionless heat-transfer area. The residence time θ and the coolant flow rate F_c are the manipulated inputs that can be used to control the composition c and reactor temperature T. The values of the process parameters are shown in Table 1.

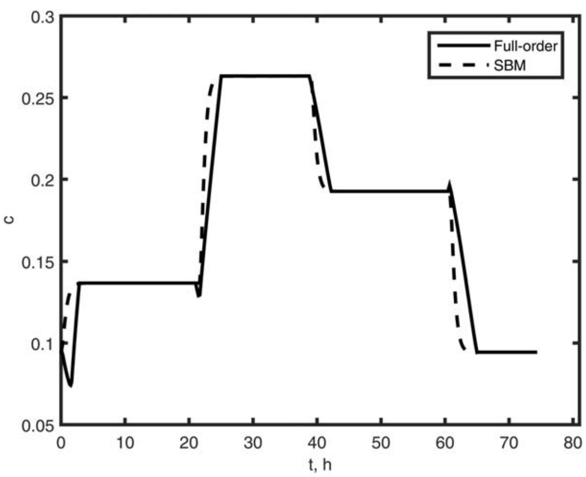

Figure 4. Evolution of the product concentration as predicted from the integrated scheduling and control calculation using the full order model (Problem P1) (solid line) and SBM (Problem P2) (dotted line).

Depending on the choice of operating conditions, the reactor can make four different product grades; the process conditions associated and quality variables **y** corresponding to each product are presented in Table 2.

The goal of the scheduling problem is to establish the production sequence and processing time for each product, such that overall profit is maximized. Previous studies[16] have indicated that the steady states corresponding to products A and B are stable, while the steady states for C and D are unstable, suggesting that control and stability considerations must be accounted for in making scheduling decisions.

Solution approach

Problems P1 and P2 were reformulated as described in the previous section and implemented in GAMS.[66] We used a discretization with $N_e = 20$ finite elements, each having $N_{\text{cp}} = 2$ collocation points. The endpoint tolerances in Equation 13d were set to $\varepsilon=0.0001$ for the full model and $\varepsilon=0.0002$ for the SBM case (the latter to account for the fact that the linear response of the closed-loop system reaches steady state asymptotically). We let $\bar{j}=20$. The parameter λ_r in Equation 5g was set to 1.001. We used the MINLP solver DICOPT,[67] with CONOPT[68] as the NLP solver and CPLEX[69] as the MIP solver. To obtain a baseline result, we began by solving Problem P1 where, for smooth inputs, the penalties ρ in Equation 14a were defined as a function of the allowable rates of change of the inputs, as

Table 3. Computational Statistics for the Solution of Problems P1 and P2 (Results Obtained on a PC Running Windows 7® 64 bit, with a 3.0 GHz Intel Core i7® Processor with 8 GB of RAM)

Problem	Equations	Continuous Variables	Binary Variables	CPU Time (s)
P1	2031	1684	16	12.57
P2	1039	1020	16	0.61

$$\rho_1=\tau_s/N_e(\lambda_2-\lambda_1)200\frac{\text{m}^3}{\text{h}^2} \quad \text{and} \quad \rho_2=\tau_s/N_e(\lambda_1-0)200\frac{\text{m}^3}{\text{h}^2}$$

for Fc, and

$$\rho_1=\tau_s/N_e(\lambda_2-\lambda_1)0.1\frac{\text{h}}{\text{h}} \quad \text{and} \quad \rho_2=\tau_s/N_e(\lambda_1-0)0.1\frac{\text{h}}{\text{h}}$$

for the input θ, with $\lambda_1=0.33$ and $\lambda_2=1$ being the collocation points. The solution suggested the production sequence $B \rightarrow D \rightarrow C \rightarrow A$, and the state and input trajectories are shown in Figure 3.

Moving on to the proposed SBM-based approach, we note that the maximum relative orders for quality variables c and T for the process (16) are $r^c=2$ and $r^T=1$. Thus, we used a second-order SBM, imposing a critically damped behavior of the form

$$\beta_c^2\frac{d^2c}{dt^2}+2\beta_c\frac{dc}{dt}+c=c_{\text{sp}} \tag{17a}$$

for the composition c, and a first-order response of the form

$$\beta_T\frac{dT}{dt}+T=T_{\text{sp}} \tag{17b}$$

for the temperature T, for each transition between products. Note that these responses are decoupled.

We then solved problem P2 using only the SBM (17a), and closed-loop time constant $\beta_c=0.4$ h. The solution of the problem provided the time-varying values of $c_{\text{sp}}(t)$ that correspond to the optimal product and product transition sequence. We then constructed the temperature setpoint signal T_{sp} by choosing the steady-state values of the temperature for each product from Table 2 and a closed-loop time constant for (17b) of $\beta_T=0.8$ h (note that this is possible because the closed-loop responses of the composition and temperature are decoupled as described above).

The solution of Problem P2 is similar to that obtained for Problem P1. The evolution of the product concentration c for the two cases is presented in Figure 4. The solution statistics are provided in Table 3. The impact of increasing the number of products (and, implicitly, the number of binary variables) is further discussed in Appendix.

Focusing then on the MPC aspects of the proposed integration strategy, the SBM (17) was implemented as a soft constraint.

The controller (18) was implemented in MATLAB[70] and solved using IPOPT[71] and the OPTI Toolbox.[72] We used a discretized version of the dynamic equations based on an implicit Euler scheme, resulting in the following expression for the MPC controller (12)

$$\begin{aligned}\min_{\mathbf{u}}\ \bar{J}_{\text{control}}=&\sum_{a=1}^{3}w_1(F_{c,a}-F_{c,a-1})^2+w_2(\theta_a-\theta_{a-1})^2\\&+w_3\left(\left.\frac{dc}{dt}\right|_a-\bar{c}_a\right)^2+w_4\left(\left.\frac{dT}{dt}\right|_a-\frac{1}{\beta_T}(T_{\text{sp},a}-T_a)\right)^2\\&\text{s.t. process model (16)}\\&\beta_c^2\frac{d\bar{c}}{dt}+2\beta_c\bar{c}+c=c_{\text{sp}}\end{aligned} \tag{18}$$

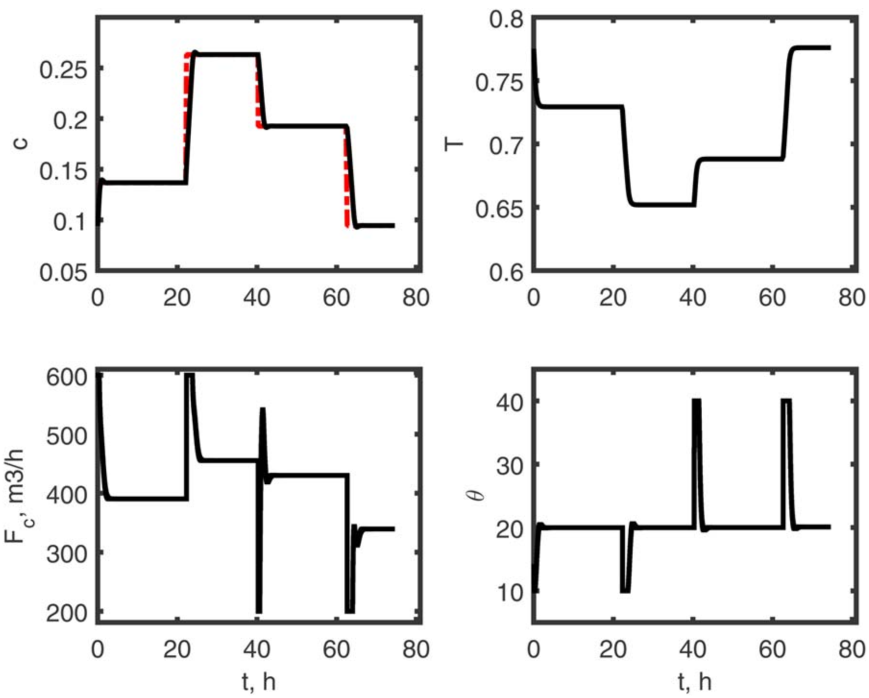

Figure 5. Evolution of quality variables and manipulated inputs of the process as computed by the scheduling-oriented model predictive controller. Top left: the stepwise setpoint for *c* is represented in dash-dot line.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

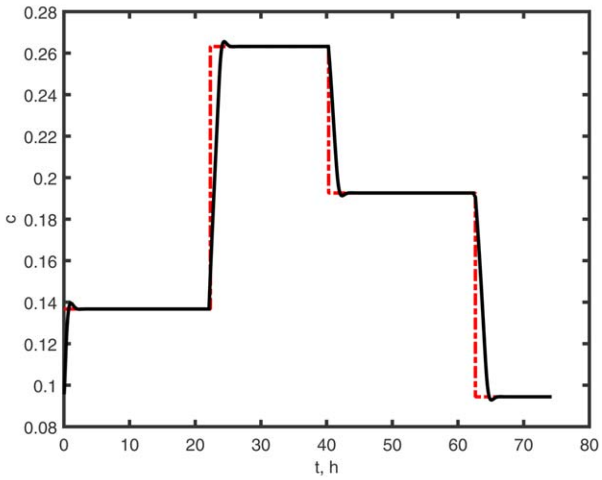

Figure 6. Evolution of product concentration *c* under scheduling-oriented MPC.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

with a sampling time of 3 min and a prediction horizon of 9 min; *a* denotes the corresponding time instants. It was verified that increasing the prediction horizon and/or reducing the sampling time did not yield significant changes in performance. $\frac{dc}{dt}|_a$ and $\frac{dT}{dt}|_a$ were computed using expressions (16), and in the expression above, $\bar{c}=dc/dt$. The controller (18) was then used to track the time-varying setpoint $\mathbf{y}_{sp}(t)$ computed from the solution of Problem P2 as described above. The simulation results are presented in Figure 5. Note that the proposed scheduling-oriented MPC imposes the desired linear responses for the composition and temperature variables. The data presented in the figure suggest that the small overshoot (see Figure 6) in the concentration response is caused by actuator saturation. In turn, this validates our choice of incorporating the SBM as a soft (rather than hard) constraint in the MPC formulation.

Results and Discussion

Economic performance

The solution of problems P1 and P2 yielded a total profit (calculated as $J_{\text{scheduling}} \cdot T_c$) of, respectively \$5470 and \$5506, with cycle times of, respectively, T_c=74.14 h and T_c=73.99 h. These values are very close, confirming the fact that the proposed low-order model captures appropriately the scheduling-relevant dynamics of the process.

Furthermore, the profit computed by evaluating the closed-loop simulation results of the system operating under SO-MPC control (Figure 5) was \$5342 for the 73.99 h cycle time, evidencing the performance of the proposed integrated scheduling and control approach. It is noteworthy that this performance is achieved on an open-loop unstable process, which attests to the benefits of implementing the schedule in closed-loop.

We also note that in the case of plant-model mismatch, the addition of integral action to the MPC formulation (e.g., as discussed by Pannocchia and Rawlings[73]; Baldea and Touretzky[74]) should be considered in order to obtain offset-free tracking of the setpoints $\mathbf{y}_{sp}(t)$.

Conclusions

In this article, we proposed a novel framework for integrating optimal production scheduling and MPC for continuous process systems. Our efforts were motivated by the need to overcome the high dimensionality and stiffness of the process models used in most existing approaches for integrating scheduling and control, and by the necessity of providing closed-loop stability in the operation of the process. Our framework is predicated on the use of a low-dimensional time scale-bridging model (SBM) that captures the closed-loop process dynamics over long time scales that are relevant to scheduling calculations. In this work, we relied on a linear model of order equal to the maximum relative order of the process. To synchronize the scheduling and MPC calculations, the SBM was incorporated in the formulation of the controller as a (soft) constraint, an approach that we referred to as scheduling-oriented MPC (SO-MPC).

We expect that the proposed framework will scale very favorably for large-scale systems (as the number of quality variables/outputs that are of interest for scheduling is typically significantly lower than the number of system states). Moreover, our framework provides desirable closed-loop stability and performance properties to the resulting integrated scheduling and control problem.

The theoretical results were illustrated with a case study, demonstrating the implementation of the framework as well as its excellent performance.

Notation

Sets

i = products
j = finite elements
k = collocation points
s = production time slots

Parameters

$c_{\text{storage},i}$ = storage cost of product i, \$/kg/h
N_{cp} = number of collocation points
N_e = number of finite elements
N_p = number of products
N_s = number of production slots
n_u = cardinality of input vector **u**
n_x = cardinality of state vector **x**
n_y = cardinality of output vector **y**
q_i = production rate of product i, kg/h
r^l = relative degree of output y
$t^p_{\max}$ = maximum production time, h
w = MPC objective function weights
R = MPC weighting matrix
Q = MPC weighting matrix
T_p = MPC prediction horizon, h
W = matrix of Radau coefficients
$\beta_{l,m}$ = tunable SBM parameter
δ_i = demand of product i, kg
$\delta_{r,i}$ = demand rate of product i, kg/h
λ_i = allowable overproduction coefficient for product i
$\lambda_{r,i}$ = allowable overproduction coefficient for product i, when demand rate is used
ε^l = tolerance for state variable l at end of transition
π_i = price of product i, \$/kg
$\omega_{\max}$ = maximum quantity of product, kg

Continuous variables

F_{cw} = cooling water flow rate, m^3/h
F_{init} = initiator flow rate, m^3/h
t^f_s = end time of slot s
t^s_s = start time of slot s

T_m = total production time, h
$\mathbf{u}$ = vector of input variables in the dynamic process model
u^l = element of vector $\mathbf{u}$
$\mathbf{x}$ = vector of state variables in the dynamic process model
x^l = element of vector $\mathbf{x}$
$\mathbf{y}$ = vector of output variables in the dynamic process model
y^l = element of vector $\mathbf{y}$
$\mathbf{y}_{sp}$ = vector of setpoints
ρ_1^l, ρ_2^l = limits of rates of change of manipulated input u^l

Positive variables

t_s^f = end time of slot s, h
t_s^s = start time of slot s, h
t_s^p = production time of slot s, h
$t_{i,s}^p$ = production time of product i in slot s, h
T_c = total production time, h
τ_s = transition time in slot s, h
ω_i = quantity of product i, kg
$\omega_{i,s}$ = quantity of product i made in slot s, kg

Binary variables

$\mathbf{z}_{i,s}$ = allocation of product i to slot s

Subscripts

sp = setpoint
ss = steady state

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Appendix

In this section, we study the impact of increasing the number of variables on the computational performance of problems P1 and P2. Specifically, we consider an extended product wheel comprising eight products. The corresponding parameters are presented in Table A1; the demand rates have been reduced compared with the four-product case (Table 2) to prevent exceeding the production capacity of the plant. We refer to the corresponding problems as problems P1* and P2*, and solve them following exactly the same paradigm we used in addressing problems P1 and P2.

Table A1. Quality Variables for Extended Product Wheel for the CSTR

Product i	$\delta_{r,i}$ (m^3)	q_i (m^3/h)	π_i ($\$/m^3$)	$c_{storage,i}$ ($\$/m^3/h$)	c_{ss}	θ_{ss} (h)
A	0.0632	1.1	180	5.0	0.0944	20
B	0.1265	1.1	110	0.5	0.1367	20
C	0.1265	1.1	60	2.2	0.1926	20
D	0.0949	1.1	140	1.05	0.2632	20
E	0.0949	1.1	180	2.5	0.1155	20
F	0.1581	1.1	180	0.25	0.1646	20
G	0.1391	1.1	70	1.1	0.22	20
H	0.1265	1.1	150	0.5	0.27	20

Table A2. Computational Statistics for the Solution of Problems P1* and P2* (Results Obtained on a PC Running Windows 7® 64 bit, with a 3.0 GHz Intel Core i7® Processor with 8 GB of RAM)

Problem	Equations	Continuous Variables	Binary Variables	CPU Time (s)
P1*	4123	3428	64	41.27
P2*	2139	2100	64	4.52

The solutions of the two problems are very similar: P1* and P2* yielded a total profit (calculated as $J_{\text{scheduling}} \cdot T_c$) of, respectively $12,517 and $12,882, with cycle times of, respectively, $T_c = 188.61$ h and $T_c = 192.27$ h. The discrepancy can potentially be explained by the fact that the optimal production sequences for the two problems ($F \rightarrow B \rightarrow H \rightarrow D \rightarrow G \rightarrow E \rightarrow C \rightarrow A$ and, respectively, $F \rightarrow B \rightarrow H \rightarrow D \rightarrow G \rightarrow C \rightarrow E \rightarrow A$) differ slightly in the order of products E and C.

The computational statistics are presented in Table A2, and suggest that our strategy scales favorably with an increase in the number of products in the product wheel (which, implicitly, leads to an increase in the number of both continuous and binary variables in the problem formulation).

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