Integration of Scheduling and Control for Batch Processes Using Multi-Parametric Model Predictive Control

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Integration of scheduling and control results in Mixed Integer Nonlinear Programming (MINLP) which is computationally expensive. The online implementation of integrated scheduling and control requires repetitively solving the resulting MINLP at each time interval. (Zhuge and Ierapetritou, Ind Eng Chem Res. 2012;51:8550–8565) To address the online computation burden, we incorporare multi-parametric Model Predictive Control (mp-MPC) in the integration of scheduling and control. The proposed methodology involves the development of an integrated model using continuous-time event-point formulation for the scheduling level and the derived constraints from explicit MPC for the control level. Results of case studies of batch processes prove that the proposed approach guarantees efficient computation and thus facilitates the online implementation. © 2014 American Institute of Chemical Engineers *AIChE J*, 60: 3169–3183, 2014
Keywords: integration of scheduling and control, event-point scheduling formulation, multi-parametric Model Predictive Control, mixed integer nonlinear programming, batch processes

Introduction

Scheduling of process operations is an important activity especially when multiple multipurpose units and a variety of products are involved to achieve the optimal production capacity and, thus, maximize plant profitability. Generally the solutions of scheduling problems involve the allocation of resources (material and equipments) at appropriate time over a production horizon following a predefined recipe for the production of specific products. For a short-term scheduling problem, the solutions are composed of equipment assignment, amount of material processed in units, task sequence, and task starting/ending times. During the past years significant efforts have been made in the development of modeling and optimization approaches for batch scheduling problems. Detailed review regarding the problem formulations and optimization methods in batch scheduling can be found in Floudas and Lin,[2] Mendez et al.,[3] Mouret et al.,[4] and Maravelias.[5]

Unlike the steady state operations in continuous processes, batch processes are operated at transient state. In batch operations, the state variables are varying under constraints stemmed from mass and energy conservation laws.[6] The task of control problem is to obtain the optimal state profiles by minimizing the operation cost under these constraints.[7] Thus, the objective of batch control problem is different from the one addressing continuous processes. For continuous processes, the units operate at steady state and the optimal control strategies are designed to reduce off-spec products during transitions between different production stages. In contrast, the objective for batch control problem is to improve the productivity during transient periods by generating optimal operating conditions.

Traditionally, production scheduling and process control problems are studied separately in chemical processes. However, there are variables that connect the scheduling and control level such as the state variables at the starting and ending of the transient periods, durations for the transient periods and amounts of material being processed in units. Therefore, scheduling and control are naturally linked and cannot be considered completely separate. Using an integrated approach that models the scheduling and control simultaneously, information is exchanged between scheduling and control level, contributing to the integrated decision making which guarantees economical process operations.[8–10]

Previous published articles in this area have demonstrated the advantages of integration. Bhatia and Biegler[11] proposed a framework for the integration of design, scheduling, and control of multiproduct batch plants. The authors addressed flowshop scheduling and replaced batch recipes with detailed dynamic models and show the improvement of profitability due to their integration using numerical examples. Mishra et al.[12] compared the performance of standard recipe approach (SRA) with the overall optimization approach (OOA) in optimizing general batch plants. In SRA, the production scheduling problem follows the basis of standardized recipes and is formulated using event-point-based continuous-time formulation proposed in Ierapetritou and Floudas,[13] whereas in OOA the dynamic models of the reaction tasks are incorporated into the state-task network (STN) framework. The OOA approach leads to a mixed integer dynamic optimization (MIDO) problem which is discretized and

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solved as a Mixed Integer Nonlinear Programming (MINLP). Their results shown that the OOA outperformed SRA in terms of profitability. Recently Nie et al.[14] used state equipment network to represent a process and formulated mixed-logic dynamic optimization for integrated scheduling and control. They demonstrated the advantages of integrated approach over conventional scheduling method through numerical results. Chu and You[15] proposed to use Benders Decomposition to decrease the computation complexity, and two-stage stochastic program[16] to handle the uncertainties in the integration of scheduling and dynamic optimization for batch processes. For sequential batch processes, Chu and You[17] modeled the dynamics of the process using Pareto frontiers that are obtained through offline recipe optimization, and integrated them with the scheduling level. The resulting integrated problem is computationally more efficient than the original MINLP. They also proposed a new online integrated method in which a reduced integrated problem is developed using a rolling horizon approach.[18]

Challenges of integration of scheduling and control for batch processes mainly lie in modeling and computation. Since scheduling and control levels have different dynamics and different time scales, the integration requires high-fidelity representations of both the scheduling problem and the dynamics of the plant.[10] Moreover, the resulting MIDO is typically nonlinear and nonconvex, and the discretized MINLP involves a large number of variables and constraints and requires excessive computation effort to get solved.[19,20] Thus, the problem complexity limits the scale of the problems that can be considered in online applications.

In this study, we propose to use multi-parametric Model Predictive Control (mp-MPC)[21] in the integration of scheduling and control, since it is capable in generating the control solution fast in the presence of disturbance by evaluating the function of predetermined explicit solution. Model Predictive Control (MPC) is an online optimization technique based on a receding horizon mode.[22] At each sample point the current state and output are measured and a constrained optimization problem is solved over a future time horizon to generate the optimal future control strategy. After the first control strategy is implemented to the process, the procedure is repeated in the following time point with the horizon moving forward. mp-MPC generates the control law as a set of explicit functions of state variables, via multiparametric programming.[23] The explicit control law can, then, be obtained offline and the online optimization is reduced to simple function evaluations. Therefore, mp-MPC results in faster application of MPC in larger scale problems.[24]

To enable the integration of scheduling and control using this idea, we first linearize the nonlinear dynamics and obtain the piecewise affine (PWA) approximation model. Then, we apply the Multiparametric Toolbox (MPT)[25] and obtain the explicit control solutions as functions of state variables. We, then, transform the explicit solutions into explicit linear constraints and incorporate them into the constraints of scheduling and obtain the integrated problem. We apply this approach in two batch processes, and the results demonstrate the feasibility and efficiency of the proposed methodology.

The rest of the article is organized as follows. The description of a general integrated model for the integration of scheduling and control for batch processes is presented in section Modeling the integration of scheduling and control for batch processes, followed by the scheme of simultaneous scheduling and control using mp-MPC in section Simultaneous scheduling and control incorporating mp-MPC. Based on that, the detailed problem formulation including constraints at both scheduling and control level and the objective are presented in section Problem formulation. Two batch processes are studied using the proposed approach and results are discussed in section Case studies, and finally conclusions of our study are made in section Discussion and conclusions.

Modeling the Integration of Scheduling and Control for Batch Processes

As outlined in the introduction section, scheduling and control are modeled simultaneously in this study. The dynamic behavior of batch processes is incorporated into the constraints of scheduling problem to form an integrated problem.

The scheduling problems for batch processes typically involve decisions associated with equipment assignment, amount of material used in each task, task sequence, and task starting/ending times. The constraints are mainly composed of precedence constraints, duration of tasks, mass balance in units, and demand fulfillment. Because infinite amount of raw material is assumed in our case studies, there are no constraints on raw material availability. A general mathematical model of the scheduling problem can be concisely presented as follows

$$\max_{w,y,V,T} J(w,y,V,T) \tag{1}$$

$$s.t. \begin{cases} g_1(w,y,V,T) \geq \text{demand} \\ g_2(y) \geq \text{Constant} \\ V_{\text{in}} = V_{\text{out}} \\ T_f = T_i + T_s \end{cases} \tag{2}$$

where the vectors w and y stand for task and equipment assignment with respect to time slots or event points, respectively; V is the vector of amount of material used in different tasks; and T is the vector of processing times for tasks. The first constraint is to satisfy the demands and the second represents the task and unit assignments at slots or event points. The other two sets of constraints correspond to mass balances and duration constraints for each task or unit. The objective $J(w,y,V,T)$ is to maximize the profit over a given time horizon.

The control problem focuses on the dynamic profile of tasks in batch processes. Constraints involve the material and energy balances, initial and end values as well as bounds of state and manipulated variables in each task, during processing. Optimal control strategies are desirable as they generate transient profiles of state variables which are economically preferable. An appropriate control strategy is effective in improving the conversion or selectivity as well as saving raw materials and utility cost. A general form of the optimal control problem is as follows

$$\max_{u(t)} J(x(t),u(t),q(t)) \tag{3}$$

$$s.t. \begin{cases} \dot{x}(t) = f(x(t),u(t),V,t) \\ q(t) = h(x(t),u(t),V,t) \\ (x(t),u(t),q(t)) \in \Omega_{xuq} \\ 0 \leq t \leq T \end{cases} \tag{4}$$

where $x(t)$ is the vector of state variables such as concentration, temperature and reaction rate; $u(t)$ is the set of manipulated variables such as heating or cooling flow rate; $q(t)$ is the set of output (i.e., controlled variables) like conversion. Note that all these variables are changing with respect to time. Ω_{xuq} is the set of bounds for $x(t)$, $u(t)$, and $q(t)$. As safety is a priority, we enforce bound constraints for state variables, for example, temperature cannot exceed the upper bound. Vector V is the amount of raw materials involved in the reactions; and T is the processing time which can be either a variable or a known value provided by the scheduling level.

With simultaneous modeling, dynamic models are incorporated into the constraints of scheduling problem giving rise to the following integrated model

$$\max_{w,y,V,T,u(t)} J(w,y,V,T,x(t),u(t),q(t)) \tag{5}$$

$$s.t. \begin{cases} g_1(w,y,V,T) \geq \text{demand} \\ g_2(y) \geq \text{Constant} \\ V_{\text{in}} = V_{\text{out}} \\ T_f = T_i + T_s \\ \dot{x}_i(t) = f_i(x_i(t), u_i(t), V_i, t) \\ q_i(t) = h_i(x_i(t), u_i(t), V_i, t) \\ (x_i(t), u_i(t), q_i(t)) \in \Omega_{xuq} \\ 0 \leq t \leq T_i \end{cases} \tag{6}$$

where index i represents time slots or event points, depending on whether time slots formulation or event-point formulation is adopted in the scheduling problem, V_i and T_i are the linking variables between the scheduling and control problems. The integration of scheduling and control levels results in an overall optimization problem incorporating all the constraints and an objective function that takes into account all the decision variables in scheduling and control level, resulting in a better overall performance.

Simultaneous Scheduling and Control Incorporating mp-MPC

With integration of scheduling and control, the resulting MINLP is generally computational very expensive. In the literature to achieve better computational performance, Terrazas-Moreno et al.[26] applied Lagrangean decomposition to the integrated model and developed an iterative strategy between a master scheduling problem and a primal control problem. Their approach is effective in lowering computation time and achieving optimality of the integrated problem. Chu and You[27] used generalized Bender decomposition to solve the MIDO of the integrated problem and observed significant reduction of computation time. In Zhuge and Ierapetritou (submitted), we explore the structure of the integrated optimization problem for continuous and batch processes cyclic production, and establish an efficient decomposition scheme in which the production sequence could be separated from the integrated problem when certain conditions are satisfied.

As described in the previous section, the online implementation of integrated scheduling and control requires a repetitive solution of the resulting MINLP.[1] In this study, we propose to use mp-MPC to not only reduce the complexity of the integrated problem but also reduce the calculation in online application.

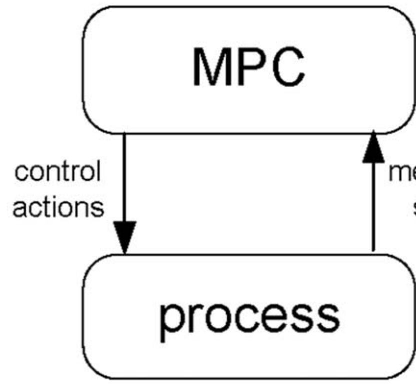

Figure 1. The working mode of conventional MPC.

A brief summary of the parametric programming is provided here which serves as a basis for mp-MPC. Problem (7) describe a parametric programming problem which obtains the objective z as a function of parameters x, and Eq. 8 describes the corresponding critical regions

$$\begin{aligned} z(x) &= \min_u f(u,x) \\ s.t.\ & g(u,x) \leq 0 \\ & x \in \Omega_x \\ & u \in \Omega_u \end{aligned} \tag{7}$$

$$\begin{aligned} &\begin{cases} z(x) = z^i(x) \\ u(x) = u^i(x) \end{cases} \text{when } x \in \Omega_x^i \\ &\bigcup_i \Omega_x^i = \Omega_x \\ &\Omega_x^i \cap \Omega_x^j = \varnothing \end{aligned} \tag{8}$$

The solution set of parametric programming includes the objective and decision variables as a function of the parameters and the partition of the space of parameters. A certain partition produces critical regions where the optimal solutions are valid. According to the features of the objective and constraints the parametric programming problem can be categorized as mp-LP,[28,29] mp-MIQP,[30] mp-MILP,[31] mp-MINLP,[32] and mp-NLP.[33]

MPC is widely recognized as it is capable to repetitively solve the optimization problem that accounts for a future horizon in online application (Figure 1).[22] mp-MPC conversely parameterizes the states and solves the optimization problem in MPC using parametric programming and performs function evaluation in online application (Figure 2).[23,34] In a sense mp-MPC transfers the online computation into offline computation, effectively reducing the computational burden in online application.

In this work, we apply mp-MPC in the online implementation for the simultaneous solution of scheduling and control, and solve the mp-MPC problem using MPT toolbox.[25] As shown in Figure 3 the dynamic optimization at the control level is solved offline using MPT toolbox. The obtained explicit control solutions are incorporated into scheduling problem, resulting in a simplified integrated problem, that is, a MINLP whose nonlinearity only present in the objective.

Specifically four steps are involved in implementing this approach.

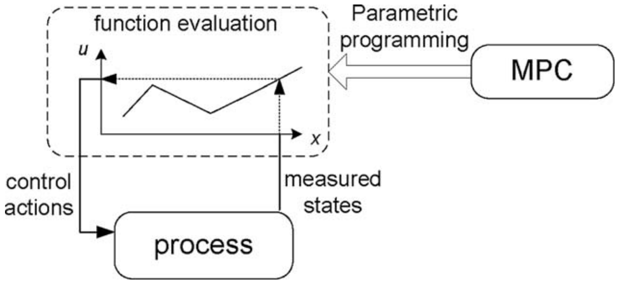

Figure 2. The working mode of mp-MPC.

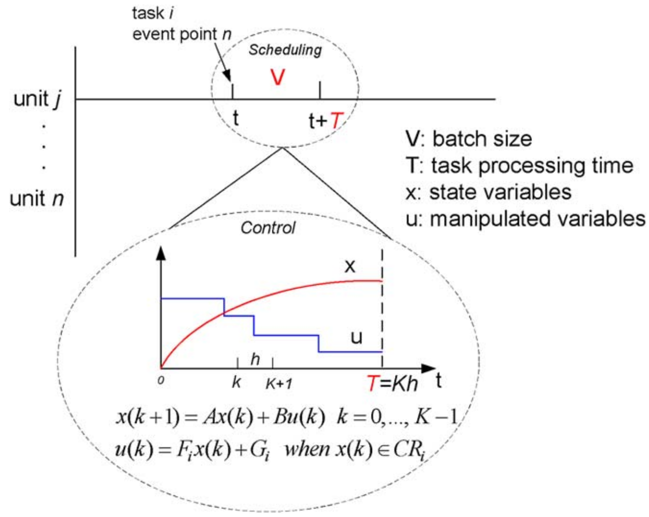

Figure 4. Demonstration of the integration using event point-based scheduling formulation.

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

Step 1: Linearize the original dynamic model using PWA approximation, which is a common approximation for Lipschitz continuous nonlinear dynamics.[35,36]

Step 2: Solve the control problem for the derived PWA using MPT toolbox and obtain the explicit solutions for the control problem.

Step 3: Transform the explicit solutions into explicit linear constraints by introducing additional variables.

Step 4: Incorporate the constraints obtained in Step 3 into the constraints of scheduling problem and build an overall economic objective, which is calculated as the revenue minus raw material and utility costs.

Problem Formulation

Figure 4 demonstrates how the scheduling and control level are connected and how they are integrated. Let us assume that task i is executed in unit j at event point n. The dynamic behavior of the manipulated variables u and state variables x are the focus of the control problem. It can be observed that the amount of material V and processing time T are shared as common variables at scheduling and control levels. Therefore, it is essential to integrate these two levels and handle the shared information simultaneously.

Constraints at scheduling level

The scheduling model follows the event-point-based formulation proposed by Ierapetritou and Floudas.[13] The model involves the constraints that are described below.

Allocation Constraints. For each event point n, only one task can take place in unit j if unit j is suitable for task, that is, $i \in I_j$ $y(j,n)=1$ indicates that unit j is utilized at event point n. If $y(j,n)=0$, then all $w(i,n)$ are forced to be zero, that is, neither task nor unit is assigned in event point n

$$\sum_{i \in I_j} w(i,n) = y(j,n), \forall j \in J, n \in N \tag{9}$$

Capacity Constraints. The material undertaken in the unit should be greater than the minimum requirement of

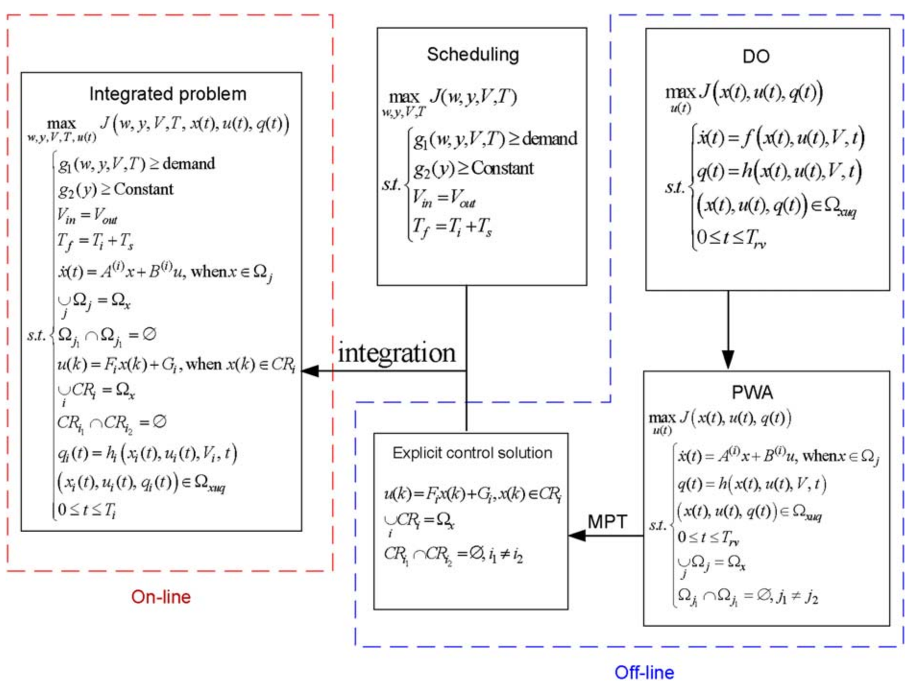

Figure 3. A scheme of integrated scheduling and control using MPT toolbox.

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

material and meanwhile less than the capacity of the unit. For a trivial case, if $w(i,n) = 0$, then $B(i,j,n) = 0$, and the following inequality still hold

$$V_{ij}^{\min} w(i,n) \le V(i,j,n) \le V_{ij}^{\max} w(i,n), \forall i \in I, j \in J_i, n \in N \tag{10}$$

Storage Constraints. The intermediate material at any state stored in storage tank at event point n is limited by the tank capacity. In the case that unlimited intermediate storage is assumed, $\mathrm{ST}\,(s)^{\max}$ goes to infinity

$$\mathrm{ST}\,(s,n) \le \mathrm{ST}\,(s)^{\max}, \forall s \in S, n \in N \tag{11}$$

Material Balance. The amount of material of state s at event point n is equal to the sum of the material amount at the previous event point and the amount produced at the previous event point subtracted by the amount delivered to the market and amount consumed by the unit at the current event point

$$\begin{aligned} \mathrm{ST}\,(s,n) = {} & \mathrm{ST}\,(s,n-1) - d(s,n) + \sum_{i \in I_s} \rho_{si}^{p} \sum_{j \in J_i} V(i,j,n-1) \\ & - \sum_{i \in I_s} \rho_{si}^{c} \sum_{j \in J_i} V(i,j,n), \forall s \in S, n \in N \end{aligned} \tag{12}$$

Duration Constraints. The processing time of task i at unit j is calculated as the sum of a fixed term α_{ij} and a varying term $\beta_{ij} V(i,j,n)$ which is linearly increasing with the amount of material

$$\begin{aligned} T^{\mathrm{f}}(i,j,n) = T^{\mathrm{s}}(i,j,n) + \alpha_{ij} w(i,n) + \beta_{ij} V(i,j,n), \\ \forall i \in I, j \in J_i, n \in N \end{aligned} \tag{13}$$

When the process dynamics are integrated, the processing time of tasks (T_{rv}) should be variables as shown in (14) rather than a proportional term in (13)

$$\begin{aligned} T^{\mathrm{f}}(i,j,n) = T^{\mathrm{s}}(i,j,n) + \alpha_{ij} w(i,n) + T_{rv}(i,j,n) y(j,n), \\ \forall i \in I, j \in J_i, n \in N \end{aligned} \tag{14}$$

Sequence Constraints: Same Task in the Same Unit. Task i starting at event point $n+1$ should start after the end of the same task processed at unit j but started at event point n. If $w(i,j) = y(i,j) = 0$, (15) is trivially satisfied

$$\begin{aligned} T^{\mathrm{s}}(i,j,n+1) \ge T^{\mathrm{f}}(i,j,n) - H(2 - w(i,n) - y(j,n)), \\ \forall i \in I, j \in J_i, n \in N, n \ne N \end{aligned} \tag{15}$$

$$T^{\mathrm{s}}(i,j,n+1) \ge T^{\mathrm{s}}(i,j,n), \forall i \in I, j \in J_i, n \in N, n \ne N \tag{16}$$

$$T^{\mathrm{f}}(i,j,n+1) \ge T^{\mathrm{f}}(i,j,n), \forall i \in I, j \in J_i, n \in N, n \ne N \tag{17}$$

Sequence Constraints: Different Tasks in the Same Unit. Task i starting at event point $n+1$ in unit j should start after the end of the other tasks processed at unit j but started at the prior event point

$$\begin{aligned} T^{\mathrm{s}}(i,j,n+1) \ge T^{\mathrm{f}}(i',j,n) - H(2 - w(i',n) - y(j,n)), \\ \forall i \in I_j, i' \in I_j, i \ne i', j \in J, n \in N, n \ne N \end{aligned} \tag{18}$$

Sequence Constraints: Different Tasks in Different Units. Tasks starting at event point $n+1$ should start after the end of tasks starting at event point n, for whichever units the tasks are processed in

$$\begin{aligned} T^{\mathrm{s}}(i,j,n+1) \ge T^{\mathrm{f}}(i',j',n) - H(2 - w(i',n) - y(j',n)), \\ \forall j, j' \in J, i \in I_j, i' \in I_j, i \ne i', n \in N, n \ne N \end{aligned} \tag{19}$$

Sequence Constraints: Completion of Previous Tasks. Task should start after all the previous tasks in the same unit are finished

$$\begin{aligned} & T^{\mathrm{s}}(i,j,n+1) \ge \sum_{n' \in N, n' < N} \sum_{i' \in I_j} (T^{\mathrm{f}}(i',j,n') - T^{\mathrm{s}}(i',j,n')), \\ & \forall i \in I, j \in J_i, n \in N, n \ne N \end{aligned} \tag{20}$$

Time Horizon Constraints. The starting time and ending time for each task should be within the time horizon

$$T^{\mathrm{f}}(i,j,n) \le H, \forall i \in I, j \in J_i, n \in N \tag{21}$$

$$T^{\mathrm{s}}(i,j,n) \le H, \forall i \in I, j \in J_i, n \in N \tag{22}$$

Constraints at control level

The control strategy in batch processes involves generating time-varying profiles of manipulated and state variables. For example, when a batch reactor is in operation temperature plays an important role in affecting reaction rate and conversion. To achieve high conversion as well as reduce the heating or cooling utility cost, a comprehensive objective involving the process yield and utility cost is usually adopted.

A first principle model based on material and energy balances describes the system dynamic of batch process. The state variables include concentration, temperature, and pressure; the manipulated variables are heating or cooling flow rate, and feeding flow rate in semibatch processes. Following is a general form of such a model

$$\begin{aligned} \dot{x}(t) &= f(x(t), u(t)) \\ q(t) &= h(x(t), u(t)) \\ x(0) &= x_0, u(0) = u_0 \end{aligned} \tag{23}$$

where x represents the vector of state variables, q is the output, and u is the vector of manipulated variables.

During batch operations the process variables are undergoing transient state. Therefore, unlike the continuous case in which an optimal constant set-point is obtained, the objective in batch operation is to determine the optimal transient profile which maximizes or minimizes an economic performance including revenue, material cost, and utility cost.

A general form of objective function is

$$\max_{u(t)} J = \Phi(x(t_{\mathrm{f}})) + \int_0^{t_{\mathrm{f}}} L(x(t), u(t)) dt \tag{24}$$

where J is the overall profit to be maximized, t_{f} is final time; and Φ is the profit at the final time point. The integral term is a comprehensive form involving the profit due to production and the utility cost with respect to the entire transient period.

Constraints including the process dynamics (23) as well as safety constraints including bounds for temperature and other important state variables (25), and unit operation specifications such as the maximum valve position

$$x_{\min} \leq x(t) \leq x_{\max}$$
$$u_{\min} \leq u(t) \leq u_{\max} \tag{25}$$

The linking variables and constraints

After solving the mp-MPC problem we obtain the state transitions at each sample step Eqs. 26–28 and the manipulated variables as linear functions of the states Eqs. 29–31. These constraints describe the dynamic profiles of manipulated variables and state variables.

PWA Approximation of the Kinetic Model.

$$x(k+1)=A_jx(k)+B_ju(k)+C_j,\quad \text{if } x(k) \in \Omega_j, k \in K=\{1,2,...,N_K\} \tag{26}$$

where

$$\Omega_j=\{x : V_jx \leq W_j\}, j \in J=\{1,2,...,N_J\} \tag{27}$$

and Ω_j satisfies the following conditions which enforce that $\{\Omega_1, \Omega_2, \ldots, \Omega_{N_J}\}$ represents a complete and nonoverlapping partition of Ω_x

$$\bigcup_j \Omega_j=\Omega_x$$
$$\Omega_{j_1} \cap \Omega_{j_1}=\emptyset, j_1, j_2 \in J \text{and } j_1 \neq j_2 \tag{28}$$

Explicit Control Solutions Obtained by Solving mp-MPC Problem Using the MPT Toolbox.

$$u(k)=F_ix(k)+G_i, \text{if } x(k) \in \mathrm{CR}_i, k \in K \tag{29}$$

where

$$\mathrm{CR}_i=\{x : H_ix \leq K_i\}, i \in I=\{1,2,...,N_I\} \tag{30}$$

and CR_i satisfies the following constraints

$$\bigcup_i \mathrm{CR}_i=\Omega_x$$
$$\mathrm{CR}_{i_1} \cap \mathrm{CR}_{i_2}=\emptyset, i_1, i_2 \in I \text{and } i_1 \neq i_2 \tag{31}$$

Equations 26–31 are implicitly linear, because the linear functions are valid in certain regions. We need to transform them into explicit linear constraints Eqs. 32–37.

Binary variables $y1$ are introduced to select the critical region in (30). If $y1_i=1$ this means that x is located in region i while if $y1_i=0$ x is not at this region. M is a big positive number which relaxes constraints inequality (32) when $y1_i=0$. Constraint (33) enforces that only one region is valid for a certain pair of H_i, K_i

$$-M(1-y1_i)+H_ix(k) \leq K_i \tag{32}$$

$$\sum_i y1_i=1 \tag{33}$$

Using these binary variables, (29) is transformed into the following constraint

$$F_ix(k)+G_i-M(1-y1_i) \leq u(k) \leq F_ix(k)+G_i+M(1-y1_i) \tag{34}$$

Similarly variables $y2$ are introduced to select the region (27) where the specific linearization is valid

$$-M(1-y2_j)+V_jx(k) \leq W_j \tag{35}$$

$$\sum_j y2_j=1 \tag{36}$$

(26) is then transformed into the following

$$A_jx(k)+B_ju(k)+C_j-M(1-y2_j) \leq x(k+1) \leq A_jx(k)+B_ju(k)+C_j+M(1-y2_j) \tag{37}$$

Since the dynamic period is discretized, the processing time T_{rv} can be calculated in Eq. 38 where h is the step length, and N_k is the total number of steps

$$T_{rv}=N_kh \tag{38}$$

Both manipulated and state variables are confined by their corresponding bounds in inequalities (39).

$$u_{\text{low}} \leq u \leq u_{\text{up}}$$
$$x_{\text{low}} \leq x \leq x_{\text{up}} \tag{39}$$

Note that all the derived constraints at control level and the constraints at scheduling level are linear. Thus, the integrated problem is simplified from the original MINLP.

The objective of the integrated problem

The objective of the integrated problem is to maximize the overall profit by obtaining the optimal scheduling and control solutions. Thus, the objective corresponds to revenue minus raw material and utility cost as follows

$$J=C^{\mathrm{P}}VX(k)-C^{\mathrm{r}}V-C^{\mathrm{u}}V\sum_{k'=1}^{k-1} u(k') \tag{40}$$

where X is the conversion, u is the scaled temperature corresponding to utility consumption,[14] $C^{\mathrm{P}}, C^{\mathrm{r}}, \text{and } C^{\mathrm{u}}$ are the product price, raw material price, and utility price, respectively.

The dynamic model is discretized with fixed step size as shown in Figure 5, and in the control problem the optimal number of steps is determined. Note that the index k in (40) is a decision variable and X and u are defined over k, making k an implicit decision variable. To eliminate this complexity, we introduce an alternative formulation given by Eq. (41) that eliminates index k from the objective using varying step size h and fixed number of steps N_k, as shown in Figure 6. The number of sample points N_k is constant and the step size h_1 and the processing time T_1 are variables. Figure 6 demonstrates two cases with different processing times but identical number of sample steps. It can be observed that a varying step size enables a flexible processing time with a constant sample size. Therefore, solving the integrated problem generates the optimal step size and the corresponding processing time

$$J=C^{\mathrm{P}}VX(N_k)-C^{\mathrm{r}}V-C^{\mathrm{u}}V\sum_{k'=1}^{N_k-1} u(k') \tag{41}$$

Case Studies

In this section, we consider two case studies that have been extensively studied in the scheduling literature and compare the results of the integrated methodology presented above with the approach that considers the scheduling and control problems separately. In this later approach, we solve the scheduling problem first and then solve the control problem based on the solution of the scheduling problem. The overall objective for the optimization problem is the maximization of profit, which is defined as the revenue from selling the products minus raw material cost, equipment cost, and

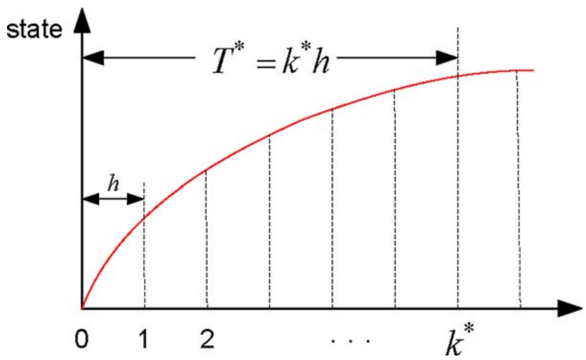

Figure 5. Discretization with fixed step size.

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

utility cost. The recipe and dataset of the case studies are the ones used at Ierapetritou and Floudas.[13]

A simple batch process

As shown in Figure 7, a batch process produces a single product through three consecutive processing stages, that is, mixing, reaction, and separation. The process is represented by the STN in Figure 8. Information regarding the capacity of units, suitability, price of material is provided in Table 1. In this case, No Intermediate Storage and Zero Wait policies are assumed.

In this study, a simplified reaction kinetic is assumed. u is a scaled temperature which is defined to substitute the rate constant and (42) is an approximation of the kinetic model.[14] The utility consumption is equal to an integral of u with respect to time. In this case, the reaction is assumed to be endothermic, so higher temperature drives the concentration of reactants to decrease fast, as indicated in (42)

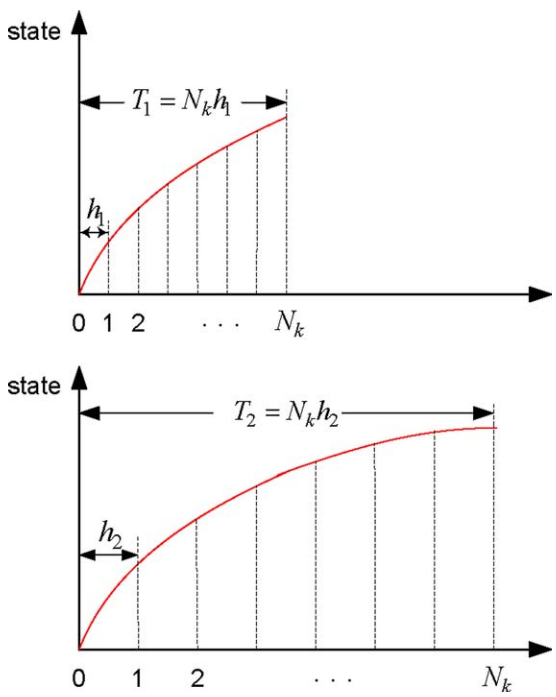

Figure 6. Discretization with varying step size but fixed number of steps.

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

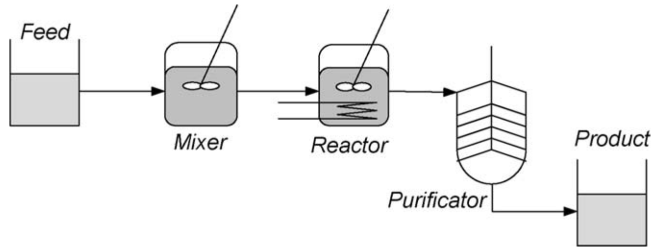

Figure 7. Flow sheet for example 1.

$$\frac{dx}{dt} = -ux \tag{42}$$

As mentioned in section Simultaneous scheduling and control incorporating mp-MPC, we transform the nonlinear model into PWA as follows.

Let $f(u,x) = dx/dt$, and linearize it at $x = x_0, u = u_0$

$$\begin{aligned}\frac{dx}{dt} &= f(u,x)\\ &= f(u_0,x_0) + (u-u_0)f_u(u_0,x_0) + (x-x_0)f_x(u_0,x_0)\\ &= -x_0u - u_0x + u_0x_0\end{aligned} \tag{43}$$

$dx/dt = (x(k+1) - x(k))/h$, where h is the sample step. Thus, we obtain

$$\frac{x(k+1)-x(k)}{h} = -x_0u - u_0x + u_0x_0 \tag{44}$$

leading to the following equation

$$x(k+1) = (1-u_0h)x(k) - x_0hu(k) + u_0x_0h \tag{45}$$

which pertains to the general form as follows

$$x(k+1) = Ax(k) + Bu(k) + C \tag{46}$$

In this case, we linearize the dynamic around seven points: $u_0 = 1$, $x_0 = [3, 2.5, 2, 1.5, 1, 0.5, 0]$.

Handle the nonlinearity brought by h. For a control problem with fixed sample step h, (45) corresponds to a linear problem. However, in this study we consider the unit processing time as a variable (T_{rv} in (14) and T_1, T_2 in Figure 6) and as we use fixed number of sample points (Figure 6), the sample step is also a variable which transforms (46) to a nonlinear equation.

From (45) and (46), we obtain

$$\begin{aligned}A &= 1 - u_0h\\ B &= -x_0h\\ C &= u_0x_0h\end{aligned} \tag{47}$$

To avoid the nonlinearity in (46), we discretize h as shown in Figure 9 and introduce binary variables to represent the selection of h.

Equations (48) and (49) represent the selection of h in the discretized segment

$$-M(1-y3_m) + H3_mh \le K3_m \tag{48}$$

$$\sum_m y3_m = 1 \tag{49}$$

Therefore, (37) is transformed into (50)

Figure 8. State-task network of example 1.

$$
\begin{aligned}
&(1-u_0hh_m)x(k)-x_{0j}hh_mu(k)+u_0x_{0j}hh_m \\
&\quad -M(1-y2_j)-M(1-y3_m) \le \\
&x(k+1) \le (1-u_0hh_m)x(k)-x_{0j}hh_mu(k)+u_0x_{0j}hh_m \\
&\quad +M(1-y2_j)+M(1-y3_m)
\end{aligned}
\tag{50}
$$

Handle the nonlinearity in (14). As in (14) both T_{rv} and y are decision variables, the last term corresponds to a bilinear term. To eliminate the nonlinearity we introduce an alternative form as follows

$$T^{\mathrm{f}}(i,j,n)=T^{\mathrm{s}}(i,j,n)+\alpha_{ij}w(i,n)+T_{rv}(i,j,n) \tag{51}$$

$$\underline{T}y(j,n) \le T_{rv}(i,j,n) \le \bar{T}y(j,n) \tag{52}$$

where $y(j,n)=1$, unit j is selected for processing and T_{rv} is subject to the lower and upper bounds. Otherwise the unit is not selected and the processing time should be zero.

The explicit control solutions generated by mp-MPC are shown in Figure 10. The integrated problem (MINLP) has 2582 variables and 17,050 constraints and it takes 218.71s to solve using GAMS/SBB[37] on a 3.0 GHz CPU/1.0 GB RAM PC. Solving the integrated problem, we obtain the dynamic profile at control level (Figure 11) and the scheduling solution in Figure 12.

A more complex batch process

As shown in Figure 13, this problem's STN represents a process that is capable of producing two products through five processing stages: heating, Reactions 1, 2, and 3, and separation of Product 2 from impure E. The material flow in this process indicates that two cascade reactions (Reaction 1 and 2) are involved in producing Product 1. It is reasonable to assume that the overall conversion is calculated by multiplying the conversions of the related reactions. The problem time horizon is 8 h. Equipment specification and price information are provided in Table 2.

Compared to the previous case, this process features cascade reactions and multiple raw materials multiple products. Thus, a product of conversions VX_1X_2 is present in the objective (53)

$$
\begin{aligned}
J=&C^{\mathrm{P}_1}V_1X_1(N_k)X_2(N_k)+C^{\mathrm{P}_2}V_3X_3(N_k) \\
&-\sum_i C^{\mathrm{r}_i}V_i-C^{\mathrm{u}}\sum_j V_j\sum_{k'} u_j(k')
\end{aligned}
\tag{53}
$$

Table 1. Data for Unit Specification and Market Information of Example 1

Unit	Capacity (L)	Suitability	Mean Processing Time (h)
Mixer	100	Task 1	4.5
Reactor	75	Task 2	3.0
Purificator	50	Task 3	1.5

State and Utility	Storage Capacity (L)	Initial Amount (L)	Price (\$/L)
State 1 (Raw)	Unlimited	Unlimited	0.2
State 2	100	0.0	0.0
State 3	100	0.0	0.0
State 4 (Product)	Unlimited	0.0	1.0
Utility	Unlimited	0.0	0.05

When building the integrated model to make the problem computationally tractable without losing essential parts of the proposed modeling approach, we made the following assumptions in this study.

Assumption 1: A generalized kinetic model that relates scaled temperature (u) and conversion (X).

A first-order reaction kinetics is assumed

$$\frac{dC}{dt}=-uC \tag{54}$$

Using the relation between concentration and conversion $C=C_0(1-X)$, we obtain

$$\frac{dX}{dt}=u(1-X) \tag{55}$$

We simplify the specific kinetic of the all the reactions and use (55) as a general form. The amounts of Products 1 and 2 are then given by VX_1X_2 and VX_3, respectively. Utility amount is equal to Vu.

Assumption 2: The conversions for the tasks, which belong to the same reaction but are executed at different reactors are equal. For example, the conversion for tasks 2 and 3 are equal. This avoids mixing the material with different conversion in storage IntBC.

Assumption 3: To satisfy the products' quality specification, we assign lower bounds for the conversion of Reactions 1, 2, and 3: $X_1>0.6$, $X_2>0.5$, and $X_3>0.3$.

In this case study, we investigate four scenarios and compare their detailed results.

Scenario 1: The integrated problem (MINLP) involving the nonlinear objective in (53) and the linear constraints shown in formula (56). This is the proposed methodology where mp-MPC is incorporated in this study

$$
\begin{aligned}
&\max_{\substack{w,y,V,d,\mathrm{ST},T^{\mathrm{s}},T^{\mathrm{f}}\\ T_{rv},x,u,X,y1,y2}} J=C^{\mathrm{P}_1}V_1X_1(N_k)X_2(N_k)+C^{\mathrm{P}_2}V_3X_3(N_k) \\
&\qquad -\sum_{i\in I_R} C^{\mathrm{r}_i}V_i-C^{\mathrm{u}}\sum_j V_j\sum_{k'} u_j(k') \\
&s.t.\begin{cases}
(9)\text{-}(12)\ \text{scheduling constraints} \\
(15)\text{-}(22)\ \text{scheduling constraints} \\
(32)\text{-}(39)\ \text{explicit MPC} \\
(48)\text{-}(50)\ \text{handle the nonlinearity in (45)} \\
(51)\text{-}(52)\ \text{handle the nonlinearity in (14)}
\end{cases}
\end{aligned}
\tag{56}
$$

Scenario 2: Directly apply the explicit control solution produced by mp-MPC to the scheduling solution generated by the pure scheduling problem in Ref. 13. In the pure

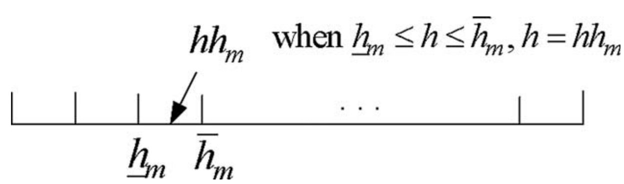

Figure 9. Discretization of step size *h*.

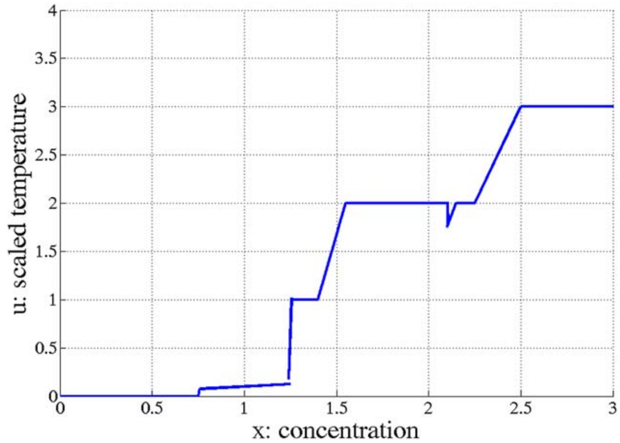

Figure 10. Explicit solution for mp-MPC.

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

scheduling problem involving constraints (9–13) and (15–22), the objective is to maximize the throughput of the process with empirical estimation of the processing time in (13). The optimization problem for Scenario 2 is presented in (57)

$$\max_{w,y,V,d,\mathrm{ST},T^s,T^f} J=\sum_n d(s=\text{``product 1''},n)+\sum_n d(s=\text{``product 2''},n) \quad (57)$$

$$s.t.\begin{cases}(9)\text{-}(13)\ \text{scheduling constraints}\\(15)\text{-}(22)\ \text{scheduling constraints}\end{cases}$$

Scenario 3: Solve the control problem using mp-MPC and apply the obtained explicit control solutions to the dynamic and obtain the operation conditions (Figures 14–16). The approximated relations are incorporated into the scheduling constraints.

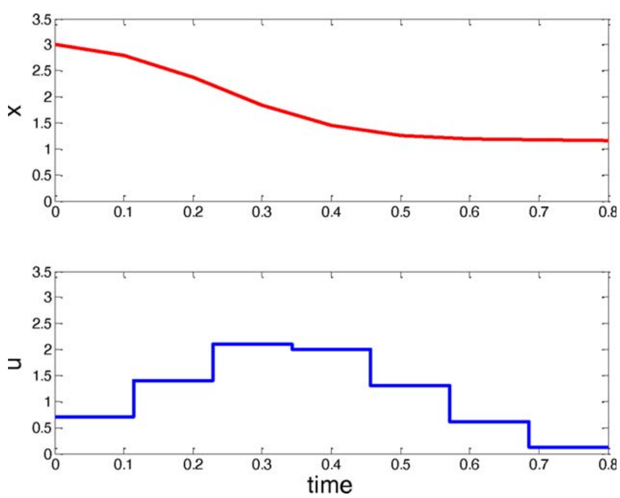

Figure 11. Dynamic profile of the reactor.

x **represents the concentration of raw material and** ***u*** **represents the scaled temperature. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]**

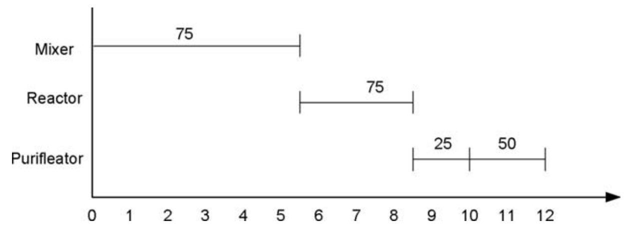

Figure 12. Scheduling solution for example 1.

From Figure 15, we obtain the empirical relation between reaction time and conversion: the required reaction time is proportional to the desired conversion

$$T_{rv}=\beta X \quad (58)$$

Thus, we have the following time constraint which replaces the original constraints in (13)

$$T^f=T^s+\alpha+\beta X \quad (59)$$

By combining the empirical relations in Figures 15 and 16, we obtain the empirical relation between utility amount and the conversion: the utility consumption is proportional to the desired conversion.

$$\text{Utility amount}=\int_0^{T_{rv}} u(t)dt=\gamma X \quad (60)$$

Based on the above, we have the optimization problem for Scenario 3

$$\max_{w,y,V,d,\mathrm{ST},T^s,T^f,X} J=C^{P_1}V_1X_1X_2+C^{P_2}V_3X_3-\sum_{i\in I_R}C^{r_i}V_i-C^u\sum_{i\in I_R}V_i\gamma X_i \quad (61)$$

$$s.t.\begin{cases}T^f=T^s+\alpha+\beta X\ \text{empirical time constraint}\\(9)\text{-}(12)\ \text{scheduling constraints}\\(15)\text{-}(22)\ \text{scheduling constraints}\end{cases}$$

This is a small scale MINLP problem which involves a nonlinear objective function and linear constraints. The formulation in (61) realizes an implicit integration (compared to the explicit integration in Scenario 1) of scheduling and control since it incorporates empirical relations of the operation conditions obtained in the control problem. Note that the implicit integration does not bring extra constraints to the scheduling problem but replaces constraint (13) with (59).

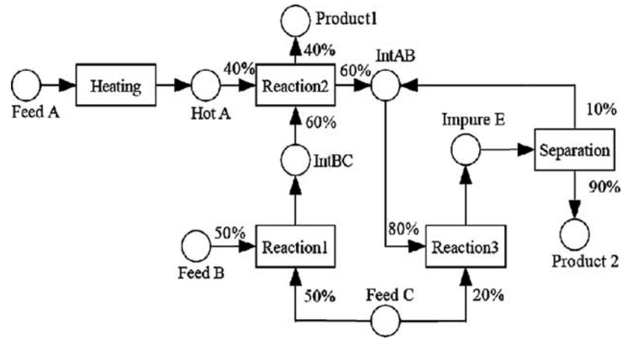

Figure 13. Flow sheet for example 2.

Table 2. Data for Unit Specification and Market Information of Example 2

Unit	Capacity (L)	Suitability	Mean Processing Time (h)
Heater	100	Heating	1.0
Reactor 1	50	Reaction 1,2,3	2.0, 2.0, 1.0
Reactor 2	80	Reaction 1,2,3	2.0, 2.0, 1.0
Distillation	200	Separation	1 for Product 2, 2 for Int AB

State and Utility	Storage Capacity (L)	Initial Amount (L)	Price (\$/L)
Feed A	Unlimited	Unlimited	0.2
Feed B	Unlimited	Unlimited	0.2
Feed C	Unlimited	Unlimited	0.2
Hot A	100	0.0	0.0
Int AB	200	0.0	0.0
Int BC	150	0.0	0.0
Impure E	200	0.0	0.0
Product 1	Unlimited	0.0	5.0
Product 2	Unlimited	0.0	1.0
Utility	Unlimited	0.0	0.05

Scenario 4: In this scenario, we build an integrated problem (MIDO) and discretize it into a MINLP using implicit Runge–Kutta method[38] which has a general form in Eqs. (62) and (63)

$$x(k+1)=x(k)+b_1K1+b_2K2+\cdots+b_sK_s \tag{62}$$

where

$$K_i=hf\left(t(k)+c_ih,x(k)+\sum_{j=1}^{s}a_{ij}K_j\right) \tag{63}$$

Here a, b, c are parameters and K is the intemediate variable. x is the state variable here it represents conversion. The dynamic model f follows the kinetic model in (55). We use Hammer-Hollingsworth with Butcher tableau as follows

$$\begin{bmatrix} c_1 & a_{11} & a_{12} & \cdots & a_{1s} \\ c_2 & a_{21} & a_{22} & \cdots & a_{2s} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & a_{s2} & \cdots & a_{ss} \\ & b_1 & b_2 & \cdots & b_s \end{bmatrix} = \begin{bmatrix} \frac{3-\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4}-\frac{\sqrt{3}}{6} \\ \frac{3+\sqrt{3}}{6} & \frac{1}{4}+\frac{\sqrt{3}}{6} & \frac{1}{4} \\ & \frac{1}{2} & \frac{1}{2} \end{bmatrix} \tag{64}$$

Thus, we obtain the following discretization of the dynamic model

$$\dot{x}(k,n)=f(x(k,n),u(k,n)),\forall k\in[1,\ldots,N_k],n\in N \tag{65}$$

$$K1(k,n)=f(t(k,n)+0.2113h(n),x(k,n)+h(n)(0.25K1(k,n)-0.0387K2(k,n)),u(k,n)) \quad \forall k\in[1,\ldots,N_k],n\in N \tag{66}$$

$$K2(k,n)=f(t(k,n)+0.7887h(n),x(k,n)+h(n)(0.5387K1(k,n)+0.25K2(k,n)),u(k,n)) \quad \forall k\in[1,\ldots,N_k],n\in N \tag{67}$$

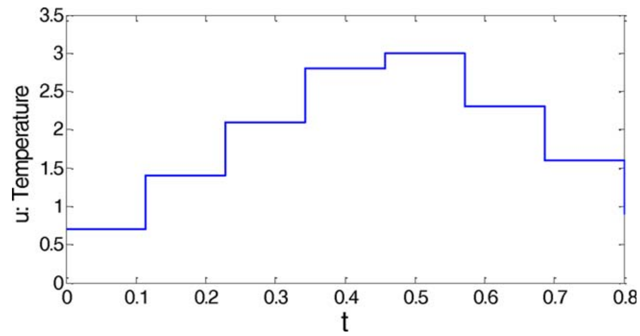

Figure 14. Temperature profile obtained by applying the explicit control solution to the reaction.

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

$$h(n)=\frac{T_{rv}(n)}{N_k} \tag{68}$$

$$x(k+1,n)=x(k,n)+h(n)(0.5K1(k,n)+0.5K2(k,n)),\forall k\in[1,\ldots,N_k-1],n\in N \tag{69}$$

The first-order derivatives of the state variables at each step are calculated using Eq. 65 and k represents sample steps in the transient duration. Through the calculation of intermediate variables $K1$, $K2$ in Eqs. 66 and 67, and the sample size in (68) the state of the next step is obtained by Eq. 69. Optimization problem for this scenario is presented in (70)

$$\max_{\substack{w,y,V,d,\mathrm{ST},T^s,T^f\\ T_{rv},x,u,X,k1,k2}} J=C^{P_1}V_1X_1(N_k)X_2(N_k)+C^{P_2}V_3X_3(N_k)-\sum_{i\in I_R}C^{r_i}V_i-C^{u}\sum_j V_j\sum_{k'}u_j(k')$$

$$s.t.\begin{cases}(9)\text{-}(12)\ \text{scheduling constraints}\\(14)\text{-}(22)\ \text{scheduling constraints}\\(65)\text{-}(69)\ \text{discretization using implicit Runge-Kutta method}\end{cases} \tag{70}$$

Scheduling solutions and detailed results of all scenarios are presented in Figures 17–21 and Table 3. Note that in the sequential solution procedures of Scenario 1, the optimization problem in (56) corresponds to MILP with the objective function being linearized using (78) and (79), whereas the optimization problem in (56) is a MINLP. For Scenario 3, the optimization problem in (61) with the objective

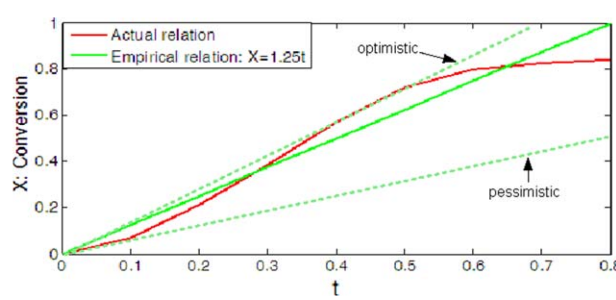

Figure 15. Conversion profile and the approximation (empirical relation).

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

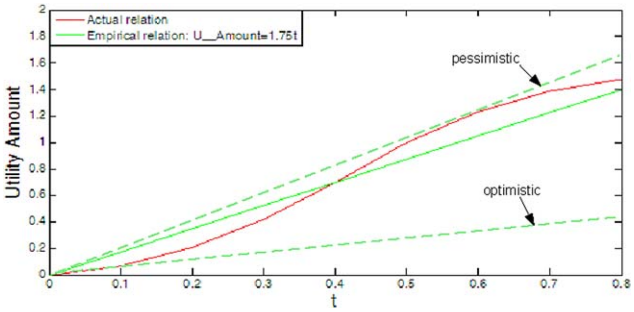

Figure 16. Utility amount profile and the approximation (empirical relation).

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

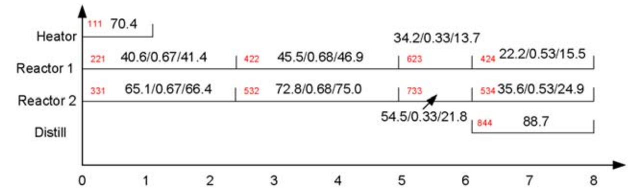

Figure 18. Scenario 2, apply control to preobtained scheduling solution.

Red number represents the index of task-unit-event point (*ijn*) and black number represents the (amount of material/conversion/utility consumption). [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

linearized using (72), (78), and (79) is a MILP, and the optimization problem in (61) corresponds to MINLP. In Scenario 4, we solve problem (70) using MINLP solver DICOPT and also the global optimizer BARON.

It can be observed that Scenario 2 generates significantly lower profit. This is due to the lack of integration of scheduling and control. In Scenario 2, the scheduling problem and control are solved sequentially, and thus, it cannot achieve the overall optimum solution since the obtained scheduling solutions based on which the control problem is solved may not be optimal for the control level. As shown in Figure 18, slots 623 and 733 which correspond to Reaction 3 correspond to smaller processing time compared to Scenario 1, resulting in less production of Product 2 (see the amount of Product 2 in Table 3) and, thus, less revenue.

It can also be observed that the profit of Scenario 3 is lower than Scenario 1 but higher than Scenario 2. The implicit integration of scheduling and control in Scenario 3 partially shares information between scheduling and control levels since it approximates the nonlinear relations using linear functions (Figures 15 and 16), so it performs better than Scenario 2 where no integration is performed but worse than the explicit integration in Scenario 1. However, the problem size of Scenario 3 is significantly smaller than Scenario 1 and thus requires much less computation time.

Table 3 also presents the detailed results for Scenario 4 where we build a MIDO for the integrated problem and discretize it into a MINLP using implicit Runge–Kutta method. There is a remarkable comparison between Scenarios 1 and 4, where they both represent the integrated problem but they differ significantly in problem size, CPU time, and profit. Although Scenario 1 (the proposed approach) has much larger problem size, it needs much less time to compute compared to DICOPT and BARON solver in Scenario 4. This is because of the problem formulation as all the constraints are linear in Scenario 1, while constraints (14), (65–69) in Scenario 4 are nonlinear. Scenario 1 produces slightly lower profit than BARON does while its solution time is reduced in nearly two orders of magnitude. Apparently DICOPT in Scenario 4 obtains a local optimum solution since in this case the profit found is 15% lower than the one using a global optimization approach.

The dash lines in Figures 15 and 16 show two extreme cases of Scenario 3 that corresponds to an optimistic and a pessimistic case. In the optimistic case, the approximated conversion profile is always above the true profile and the utility amount is lower than the true one, while in pessimistic case the approximation follows an opposite trend. Solving problem (61) for both cases results in profit \$140.29 and \$136.5, respectively. Both of them have lower profit than Scenario 3 because they use worse approximation (the distance between the linear profile and the true profile is greater) as shown in Figures 15 and 16. Note that the profit associated with Scenario 3 is obtained by incorporating the solution of problem (61)–(56) and calculating the real profit using the objective in (56), that is, the profit is the one that realized in the real case. This ensures a fair comparison between the different scenarios.

Discussion and Conclusions

Linear approximation of the objective function

The proposed formulation for simultaneous scheduling and control results corresponds to a MINLP which involves linear constraints and a nonlinear objective function. To improve the computation efficiency, we linearize the bilinear term in the objective using a simple first-order Taylor expansion (71) and, thus, transforming the problem to a MILP.

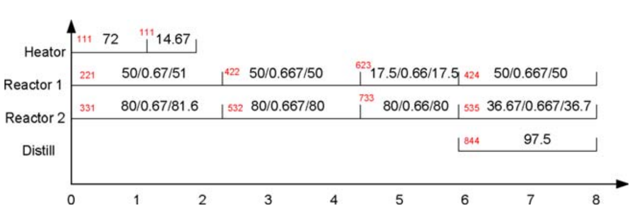

Figure 17. Scenario 1, scheduling solution for MINLP.

Red number represents the index of task-unit-eventpoint (*ijn*) and black number represents the (amount of material/conversion/utility consumption). [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

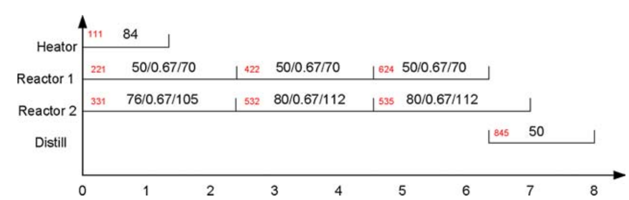

Figure 19. Scenario 3, implicit integration based on the recipe obtained in control problem.

Red number represents the index of task-unit-event point (*ijn*) and black number represents the (amount of material/conversion/utility consumption). [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

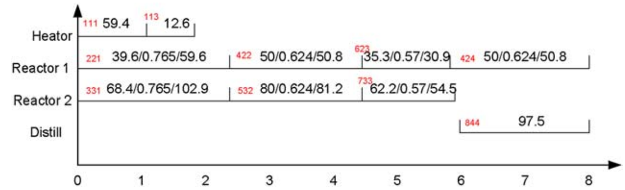

Figure 20. Scenario 4, original integrated problem MIDO discretized into a MINLP using implicit RK method, solved using GAMS/DICOPT.

Red number represents the index of task-unit-event point (*ijn*) and black number represents the (amount of material/conversion/utility consumption). [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

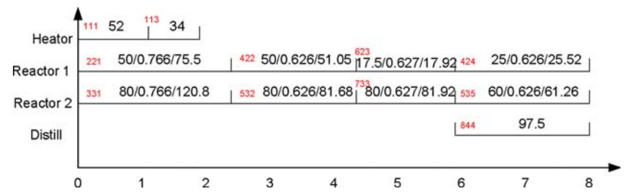

Figure 21. Scenario 4, original integrated problem MIDO discretized into a MINLP using implicit RK method, solved using GAMS/BARON.

Red number represents the index of task-unit-event point (*ijn*) and black number represents the (amount of material/conversion/utility consumption). [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

In Case 1, we linearize the term $V \times X(N_k)$ at (V_0, X_0) following (72) and obtain a linear objective function (73). We chose different points where the bilinear term is expanded and solve the corresponding MILP, and summarize the results in Table 4

$$f(u,x) \approx f(u_0,x_0)+(u-u_0)\frac{\partial f}{\partial u}(u_0,x_0)+(x-x_0)\frac{\partial f}{\partial x}(u_0,x_0) \tag{71}$$

$$VX \approx V_0X_0+(V-V_0)X_0+(X-X_0)V_0=V_0X+X_0V-V_0X_0 \tag{72}$$

$$J_0=C^P(V_0X(N_k)+VX_0(N_k)-V_0X_0(N_k))-C^rV-C^u\sum_{k'=1}^{N_k-1}u(k') \tag{73}$$

Note that the MILP is solved with a different objective (73) compared to the one of the MINLP (40). However, the results in Table 4 are calculated following the same equations as follows

$$\text{Revenue} = \text{ProductAmount} \times \text{ProductPrice} \tag{74}$$

$$\text{RawCost} = \text{RawMaterialAmount} \times \text{RawPrice} \tag{75}$$

$$\text{UtilityCost} = \text{UtilityAmount} \times \text{UtilityPrice} \tag{76}$$

$$\text{Profit} = \text{Revenue} - \text{RawCost} - \text{UtilityCost} \tag{77}$$

In Case 2 through linearization of the bilinear term in the objective (78) and (79), we obtain a linear objective function and an overall MILP problem. The derived MILP has the same problem size as the MINLP and takes around 18 s to solve using GAMS/CPLEX. The results of the MILP with four linearization points are provided in Table 5. The best linearization point is $V_1^0=V_3^0=50$, $X_1^0=X_2^0=X_3^0=0.6$ where the corresponding result \$179.96 is slightly lower than the profit of the MINLP which is \$182.55

$$V_1X_1X_2=V_1^0X_1^0X_2+V_1^0X_2^0X_1+X_1^0X_2^0V_1-2V_1^0X_1^0X_2^0 \tag{78}$$

$$V_3X_3=V_3^0X_3+X_3^0V_3-V_3^0X_3^0 \tag{79}$$

Results for both cases show that the MILP generates lower profit than the MINLP. This is because the MILP fails to capture the optimum of the original objective. However, the MILP requires significantly less computation time.

Table 3. Comparison of the Quantitative Results for Four Scenarios

Four Scenarios	Scenario 1: Integrated Problem (MINLP) Nonlinearity Only in the Objective	Scenario 2: Apply Control to Obtained Scheduling (Directly Apply Explicit Control Solution)	Scenario 3: Implicit Integration Based on the Recipe Obtained in Control Problem (Small MINLP)	Scenario 4: Original MIDO Discretized Into MINLP Using Implicit RK4 Method, Nonlinearities in the Objective and Constraints	
Problem size	16,039 variables, 107,324 constraints	N/A	653 variables, 1284 constraints	5932 variables, 8495 constraints	
Solver	Warm start solving procedures: solve MILP using CPLEX[39], and then solve MINLP using DICOPT[40], 76 s	N/A (no solver is needed)	Warm start solving procedures: solve MILP using CPLEX[39], and then solve MINLP using DICOPT[40], 14 s	DICOPT[40] 157.6 s	BARON[41] 4804.9 s, maximum CPU time is set to 6000 s
Product 1 amount (*L*)	38.71	29.77	37.70	34.38	41.25
Product 2 amount (*L*)	58.50	26.34	30.15	50.0	55.03
Revenue (\$)	252.06	175.19	218.65	221.89	261.23
Raw A amount (*L*)	86.67	70.44	84.0	72.0	86.0
Raw B amount (*L*)	65.0	52.84	63.0	54.0	85.0
Raw C amount (*L*)	84.50	70.58	73.0	73.50	84.50
Raw Cost (\$)	47.23	38.77	44.0	39.90	47.10
Utility amount (*L*)	445.47	305.60	540.40	430.76	515.60
Utility cost (\$)	22.27	15.28	27.02	21.54	25.78
Profit (\$)	182.55	121.14	147.63	160.45	188.35

Table 4. Results of the MINLP and the Derived MILP (Case 1)

	MINLP	MILP $V_0 = 50$ $X_0 = 0.5$	MILP $V_0 = 60$ $X_0 = 0.4$	MILP $V_0 = 70$ $X_0 = 0.6$	MILP $V_0 = 70$ $X_0 = 0.7$	MILP $V_0 = 40$ $X_0 = 0.7$	MILP $V_0 = 80$ $X_0 = 0.6$
Solver	SBB/IPOPT	Cplex	Cplex	Cplex	Cplex	Cplex	Cplex
ProductAmount (*L*)	53.56	45.33	43.67	51.0	51.0	51.0	45.33
Revenue ($)	53.56	45.33	43.67	51.0	51.0	51.0	45.33
RawMaterialAmount (*L*)	78.0	68.0	64.0	75.0	75.0	75.0	68.0
RawCost ($)	15.60	13.60	12.80	15.0	15.0	15.0	13.60
UtilityAmount (*L*)	42.32	40.0	41.16	20.8	20.8	20.8	40.0
UtilityCost ($)	2.12	2.0	2.06	1.04	1.04	1.04	2.0
Profit ($)	35.84	29.73	28.80	34.96	34.96	34.96	29.73

Table 5. Results of the MINLP and the Derived MILP (Case 2)

	MINLP	MILP $V_1^0=V_3^0=60$, $X_1^0=X_2^0=0.5$ $X_3^0=0.5$	MILP $V_1^0=V_3^0=60$, $X_1^0=X_2^0=0.6$ $X_3^0=0.6$	MILP $V_1^0=V_3^0=50$, $X_1^0=X_2^0=0.6$ $X_3^0=0.6$	MILP $V_1^0=V_3^0=50$, $X_1^0=X_2^0=0.5$ $X_3^0=0.5$
Solver	CPLEX for MILP, DICOPT for MINLP 76 s	CPLEX, 17 s	CPLEX, 19 s	CPLEX, 18 s	CPLEX, 18 s
Product 1 amount (*L*)	38.71	37.15	37.77	38.31	37.45
Product 2 amount (*L*)	58.5	55.82	50.14	57.38	47.61
Revenue ($)	252.06	241.55	239.02	248.93	234.84
Raw A amount (*L*)	86.67	89.07	82.4	83.1	96.1
Raw B amount (*L*)	65.0	75.3	78.63	62.07	72.36
Raw C amount (*L*)	84.5	80.23	61.12	85.13	91.79
Raw cost ($)	47.23	48.92	44.43	46.04	52.05
Utility amount (*L*)	445.47	484.0	413.8	459	349.6
Utility cost ($)	22.27	24.2	20.69	22.95	17.48
Profit ($)	182.55	168.43	173.87	179.96	165.31

This helps to achieve a balance between computation complexity and optimality as the linearization greatly simplifies the problem while keeping the solution close to the optimum.

Discussion

Chemical reactions are normally exothermic or endothermic, and therefore, temperature profile during the reactions plays a vital role in affecting the conversions. In batch process operations, as we intend to achieve high conversions with low-utility cost, it is essential to apply control to batch reactors and obtain an optimal dynamic profile for the temperature.

In this study, we model scheduling and control problem for batch processes simultaneously using mp-MPC. The reason that we adopt mp-MPC is that it generates control signal instantly by function evaluation and, thus, greatly reduce computation complexity when control level is integrated with scheduling level. To the authors' knowledge, this is the first attempt in this area to explore the possibility and feasibility of applying mp-MPC in control and scheduling problem. The main contribution of this study is that we propose a framework which is capable to transform explicit control solution generated by mp-MPC into explicit linear constraints, and incorporate with the linear constraints at scheduling level. This results in an integrated problem that involves linear constraints and a nonlinear objective. Results of case studies demonstrate that the integration achieves much high profit compared to the sequential approach.

In the case studies, we focus on single-input single-output (SISO) systems. It should be noted that in the cases of multiple-input multiple-output (MIMO) systems, the problem size of the resulting integrated problem increases, due to the fact that the number of critical regions increases exponentially in the size of the MPC problem (in terms of state dimension and prediction horizon).[42,43] For instance, a MIMO system needs more inequalities to describe the valid regions for PWA in (27) and more inequalities to represent the critical regions in (30). This requires more binary variables to select the regions and more explicit constraints to represent the selection in (32)–(37).

It should be noted that in the case studies we did not consider availability of raw materials and the demand of products. In fact we maximize the production capacity of the process following a given recipe without considering market constraints which are typically considered at planning level. Currently we use PWA system to solve mp-MPC using MPT toolbox. We believe that the progress in developing mp-MPC for nonlinear dynamic would benefit the direct integration with a nonlinear system.

This study demonstrates that mp-MPC builds linear constraints for control level and, thus, effectively reduces the complexity of the integrated problem involving scheduling and control levels. Since the integration of planning and scheduling levels results in a MILP,[44,45] we believe an integration of planning, scheduling, and control would also lead to linear constraints, if mp-MPC is incorporated. Based on this, our future efforts are toward enterprise wide optimization.

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Notation

Indices

i = tasks
j = units
s = states
n = event points
k = sample steps

Sets

I = tasks
I_j = tasks which can be performed in unit j
I_S = tasks which process state s
J_i = units which are suitable to perform task i
I_R = set of reaction tasks
N = event points within the time horizon
S = states

Parameters

$V_{ij}^{\min}$ = minimum amount of material required to process task i in unit j
$V_{ij}^{\max}$ = capacity of unit j when processing task i
$\mathrm{ST}(s)^{\max}$ = storage capacity for state s
α_{ij} = coefficient of constant part of processing time of task i in unit j
β_{ij} = coefficient of variable part of processing time of task i in unit j
H = time horizon
C^p, C^r, C^u = price of product, raw material, and utility
M = big positive number
N_k = number of discretization point

Decision variables

$w(i,n)$ = binary variable assign task i at event point n
$y(i,n)$ = binary variable assign unit j at event point n
$V(i,j,n)$ = amount of material undertaking task i in unit j at event point n
$d(s,n)$ = amount of state s sold at event point n
$\mathrm{ST}(s,n)$ = amount of state s at event point n
$T^s(i,j,n)$ = starting time of task i in unit j at event point n
$T^f(i,j,n)$ = ending time of task i in unit j at event point n
$T_{rv}(i,j,n)$ = processing time of task i in unit j at event point n
X = conversion
h = step size
x = state variables such as concentration
u = scaled temperature corresponding to utility consumption
A, B, C = coefficients in PWA model
V, W = coefficients of the inequalities corresponding to the PWA
F, G = coefficients in the explicit solution
H, K = coefficients of the inequalities describing the critical regions
CR = critical region
y_1 = binary variables selecting the critical regions
y_2 = binary variables selecting the valid regions of PWA
$K1$, $K2$ = intermediate variables in implicit RK method
Ω = domain of variables

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