

VERTICAL INTEGRATION OF PRODUCTION SCHEDULING AND PROCESS CONTROL: PROGRESS, OPPORTUNITIES AND CHALLENGES

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Abstract

Current challenges in the process industries and the pursuit of optimal operating conditions result in a need for integrating decision-making across different levels of a chemical company. Problems involving production scheduling and process control are naturally related and, if addressed simultaneously, can result in increased profits and performance. However, their integration often results in high dimensional optimization problems involving complex dynamic models for which fast solution methodologies are still unavailable. In this paper, recent developments and frameworks for the integration of scheduling and control are reviewed and compared. A case study is used to illustrate the feasibility and applicability of these frameworks, and remaining challenges and research directions are identified.

Keywords

Process control, production scheduling, integrated scheduling and control, multi-parametric model predictive control, fast model predictive control, scale-bridging models

Introduction

Dynamic market conditions and increasing pressure for competitive performance in the process industries have led to significant efforts in the pursuit of optimal operation conditions. In addition to improved process designs, these circumstances have spurred the development of strategies aimed at vertical integration and coordination of decision-making across all the layers of the chemical supply chain. Such enterprise-wide optimization efforts (Grossmann, 2005) are supported by advances in numerical optimization algorithms and by the development of modern IT tools, which allow extensive information exchange between different layers of decision-making within a company.

Progress made in integrating the upper echelons of decision-making (planning and scheduling) and the resulting benefits have provided the economic motivation and intellectual impetus for seeking integration paths further down the decision-making hierarchy, notably focusing on integrating scheduling and control. Scheduling

aims to maximize profit by setting the optimal production sequence, batch sizes, unit assignments and timing of tasks while control maximizes performance by focusing on the dynamic behavior, such as the transition between products (Zhuge & Ierapetritou, 2015). Additional motivation is provided by practical considerations related to current economic circumstances: chemical processes operate in an increasingly dynamic environment, and fast-changing prices (especially on the energy and electricity supply side) require that production schedule changes be made on a time scale comparable to the time constant of the process (Pattison, Touretzky, Johansson, et al., 2016). Under these conditions, the process may actually never reach steady state in operation and the conventionally accepted time scale separation between scheduling and control is no longer valid, making it imperative to address scheduling and control decisions in an integrated, unified way (Baldea & Harjunkoski, 2014; Du et al., 2015).

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Initial efforts towards the integration of scheduling and control followed the intuitive route of embedding the dynamic model of the process as an additional set of constraints in the scheduling problem. The result is a mixed-integer dynamic optimization problem (MIDO), and its solution provides the optimal production sequence and optimal control moves required to implement the schedule. The MIDO problem is either discretized into a Mixed Integer Nonlinear Program (MINLP) using, for example, orthogonal collocation on finite elements or implicit Runge-Kutta methods, or solved using sequential techniques. The former approach was proposed by Flores-Tlacuahuac and Grossmann (2006), and it was extended by Terrazas-Moreno et al. (2007) and Zhuge and Ierapetritou (2012), while Pattison, Touretzky, Johansson, et al. (2016) have applied the latter. The alternative of using a decoupled modelling approach, consisting of formulating the scheduling problem (master problem) as a Mixed Integer Linear Programming (MILP) and the control problem (primal problem) as Dynamic Optimization, has also been discussed. The problem is solved through iterations between the master and primal problems. Case studies have shown that the solution is close to the global optimum (Nystrom et al., 2005; Nystrom et al., 2006). Furthermore, Lagrangean and Benders decompositions have been proposed in order to reduce the computational complexity of the integrated problem, enabling online integration of scheduling and control (Chu & You, 2013a, 2013b; Terrazas-Moreno et al., 2008)

While intuitive, these developments face limitations when presented with large-scale, industry-relevant problems. In particular, solving, in a practical amount of time, mixed-integer dynamic optimization problems with high-dimensional, nonlinear and stiff constraint sets (which is typically the case for the models of chemical processes) is difficult if not impossible. In a different vein, organizational challenges pertaining to the integration of multiple disparate software systems used in a process plant and the decision making process of a company are still to be overcome (Engell & Harjunkoski, 2012).

In this work, recent developments towards efficient and fast integration of scheduling and control will be presented. The following section will present approaches for the integration of Multi-Parametric Model Predictive Control and Fast Model Predictive Control and the scheduling problem. The integrated problem using time-scale bridging models is then introduced. A case study will be used to illustrate the applicability, feasibility, advantages and disadvantages of the different methods.

Integration of scheduling and control using full scale dynamic models

Class of systems considered

We consider a generic (Baldea & Daoutidis, 2012) input-affine dynamic model of process systems of the form:

$$\begin{aligned}\dot{x} &= f(x) + G(x)u \\ y &= h(x)\end{aligned}\tag{1}$$

where x represent the state variables, u are the system inputs, y are the outputs, and f , G and h are appropriately defined vector functions. For convenience, we assume that the system is minimum phase.

Simultaneous scheduling and control incorporating mp-MPC

Model Predictive Control (MPC) makes use of an explicit model of the process to obtain a sequence of control actions by repetitively solving an optimal control problem online. At each sample point the current state and output are measured and the tracking error is minimized over a future time horizon to generate the optimal control strategy (Camacho & Bordons, 2007). The first step of the computed input trajectory is implemented to the process, and the procedure is repeated in the following time point with the horizon moving forward. MPC has been widely adopted in industry as an effective control strategy for multivariable constrained control problems (Bemporad & Morari, 2000). However, the potentially high computational effort resulting from the recurrent solution of optimization problems may limit the applicability of model predictive controllers. On the other hand, Multi-parametric Model Predictive Control (mp-MPC) arises as a solution for the computational burden, as it is capable of transferring the online computation into offline solution. mp-MPC uses multi-parametric programming techniques to obtain a set of explicit control laws, each associated to a polyhedral region in the state space (critical regions). Therefore, mp-MPC replaces the online optimization problem by simple function evaluations and allows the use of model-based controllers in a wider range of problems (Pistikopoulos, 2012).

In Zhuge and Ierapetritou (2014), a framework for the integration of scheduling and control using mp-MPC was proposed. The framework can be summarized in four steps: first, the dynamic model describing the system (1) is linearized using piecewise affine approximations (PWA). Second, the derived PWA control problem is reformulated as a parametric programming, and the explicit solutions for the control problem are obtained. Third, the explicit solutions are transformed into explicit linear constraints by introducing additional variables. Finally, the explicit constraints are incorporated into the constraints of scheduling problem, and the resulting MINLP problem can be solved for the online implementation of integrated scheduling and control.

The PWA approximations are obtained by applying the method presented in Dias et al. (2016). The resulting PWA functions will have the form of Eq. (2). In this work, the mp-MPC problem is solved using MPT toolbox (Herceg et al., 2013), and the explicit control solutions assume the form of Eq. (3). Thus the explicit constraints to be incorporated in the scheduling problem have the form of Eqs. (4)-(7).

$$x_{k+1} = A_j x_k + B_j u_k + C_j, \text{ if } x_{s,k} \in \Omega_{xi} \quad (2)$$

$$u_p = F_{i,p} x + g_{i,p}, \forall i \in S_i, p \in S_p \quad (3)$$

$$-M(1 - y_{1_{s,k,i}}) + V_i x_{s,k} \leq W_i, \forall s \in S_s, k \in S_k, i \in S_i \quad (4)$$

$$\sum_i y_{1_{s,k,i}} = 1, \forall s \in S_s, k \in S_k \quad (5)$$

$$u_{s,k} \geq F_{i,p} x_{s,k} + g_{i,p} - M(1 - y_{p,s}) - M(1 - y_{1_{s,k,i}}), \quad (6)$$

$$\forall s \in S_s, i \in S_i, k \in S_k \setminus N_k$$

$$u_{s,k} \leq F_{i,p} x_{s,k} + g_{i,p} + M(1 - y_{p,s}) + M(1 - y_{1_{s,k,i}}), \quad (7)$$

$$\forall s \in S_s, i \in S_i, k \in S_k \setminus N_k$$

where x denotes the state reference at slot s and sample step k . u denotes control inputs, and A_j , B_j and C_j are the PWA coefficients. If $y_{p,s} = 1$, product p is produced at slot s . If $y_{1_{s,k,i}} = 1$, the critical region i is selected by Eq. (4) and thus the explicit control associated with coefficients $F_{i,p}$, $g_{i,p}$ is selected through constraints (6) and (7). Equation (5) indicates that only one critical region is selected at each sample step.

In Zhuge and Ierapetritou (2014), the possibility and feasibility of using the framework for integration of scheduling and control with mp-MPC is explored. Case studies involving a batch process are presented, and the performance of the proposed model is compared to a model where a MIDO is built for the integrated problem and discretized into a MINLP using implicit Runge-Kutta method. The comparison shows that the proposed framework produces slightly lower profit while its solution time is nearly two orders of magnitude smaller. Nevertheless, the applicability of this model is limited to small and medium size control problems, provided that the number of critical regions increases exponentially as the problem size increases in terms of state dimension and prediction horizon.

Simultaneous scheduling and control incorporating Fast MPC

Fast MPC for linear systems transforms the MPC problem into a convex quadratic program, and the online computation can be sped up by exploiting the problem structure and using efficient nonlinear programming methods. Therefore, the issue of handling large-scale control problems is overcome by using Fast MPC. In Zhuge and Ierapetritou (2015), a framework involving two control loops for the integration of scheduling and control using Fast MPC is proposed. In the outer control loop, the original process dynamics is transformed into a PWA system composed by a set of Linear Time Invariant (LTI) equations and incorporated in the scheduling problem. The resulting MINLP problem is solved for the production scheduling and state references. Hereafter, the inner control loop uses Fast MPC for PWA systems to track state references provided by the outer loop. The LTI equation for current states is located using a binary search method, and the MPC problem for the selected LTI is solved using toolbox

FORCES (Domahidi, 2012), which is based on primal-dual interior-point method.

When disturbances at control level are detected, fast MPC acts to minimize state deviations. However, large disturbances may not be handled efficiently by the inner loop. Therefore, Zhuge and Ierapetritou (2015) proposed to empirically determine a threshold for state deviations, above which the state deviation would be feedback to the integrated problem and the scheduling solution would be updated.

Scheduling Problem Formulation

In this work, the problem of continuous cyclic production is addressed, and scheduling constraints are adopted from the work of Flores-Tlacuahuac and Grossmann (2006). Constraints at control level include the discretized dynamic model and bounds for state and manipulated variables. In addition, the model incorporating mp-MPC includes Eq. (4)-(7). Furthermore, the determination of the end of transition and evaluation of transition times is determined by Eq. (8)-(12).

$$x_{s,k} \geq \bar{x}_s - x_{margin} - M(1 - y_{2_{s,k}}) \forall s \in S_s, k \in S_k \quad (8)$$

$$x_{s,k} \leq \bar{x}_s + x_{margin} + M(1 - y_{2_{s,k}}) \forall s \in S_s, k \in S_k \quad (9)$$

$$\sum_k y_{2_{s,k}} \geq 1, \forall s \in S_s \quad (10)$$

$$y_{3_{s,k}} = y_{2_{s,k}} - y_{2_{s,k-1}} \forall s \in S_s, k \in S_k \setminus 1 \quad (11)$$

$$kh - M(1 - y_{3_{s,k}}) \leq \theta_s^k \leq kh + M(1 - y_{3_{s,k}}), \forall s \in S_s \quad (12)$$

Transition between slots in a continuous process naturally starts with state values set at the steady state of the previous slot, and end when the steady state value for the new product is reached. However, the duration of transition is unknown. We determine the end of transition by first dividing the transition time in k steps of duration h . We also assume that there exist some margins around the set point, and if the state is between the lower bound $\bar{x}_s - x_{margin}$ and the upper bound $\bar{x}_s + x_{margin}$, it is meeting the set point. We then introduce two binary variables, $y_{2_{s,k}}$ and $y_{3_{s,k}}$. If $y_{2_{s,k}} = 1$, the state value at step k and slot s is between the desired margins of production. If $y_{3_{s,k}} = 1$, the current value of state $x_{s,k}$ meets the quality bounds, but the previous value $x_{s,k-1}$ did not meet the quality bounds. Therefore, the transition has ended and the transition time is determined as kh by constraint (12).

Time Scale-Bridging Models for the Integration of Production Scheduling and Process Control

As shown earlier in the paper, dimensionality reduction is a key ingredient for improving the tractability of integrated scheduling and control problems. In this section, we review previous efforts predicated on obtaining a low-order model of the *closed-loop* behavior of the process, which captures its scheduling-relevant input-output dynamic behavior, and

is then embedded in the scheduling calculation. These constructs, referred to as scale-bridging models (SBMs) were initially proposed by Du et al. (2015), with extensions to MPC controllers and data-driven models introduced by Baldea et al (2016) and Pattison, Touretzky, Johansson, et al. (2016) respectively. The notion of scheduling-relevance reflects the fact that not all state and output variables x and y are relevant (or needed) for establishing the optimal schedule. Intuitively, the subset of states and/or outputs whose dynamics should be accounted for when computing the schedule (and thus captured in the SBM) includes product purities and production rates, as well as the (state) variables that are critical to the safe operation of the process and that are at or close to their constraints/bounds either during steady-state operation or during transitions (Pattison, Touretzky, Johansson, et al., 2016). Case studies carried out on industrial-scale problems (Pattison, Touretzky, Harjunkoski, et al., 2016) suggest that in practical circumstances the dimensionality of the SBM may be quite small, and significantly lower than the dimension of the first-principles model of an industrial facility.

In the general case, SBMs are of the form:

$$\begin{aligned}\hat{y} &= f_y(\hat{y}_{sp}, \hat{y}, \hat{x}, \hat{u}) \\ \hat{x} &= f_x(\hat{y}_{sp}, \hat{y}, \hat{x}, \hat{u}) \\ \hat{u} &= f_u(\hat{y}_{sp}, \hat{y}, \hat{x}, \hat{u})\end{aligned}\quad (13)$$

where the hat denotes scheduling-relevant variables, and the subscript sp refers to the target values of the scheduling-relevant process outputs, as determined by the scheduling calculation. The model representation (13) can then be embedded in the scheduling problem formulation as described above in order to capture the process dynamics.

However, closed-form representations for both output, state and input dynamics of the type (13) are difficult to obtain in the general case. In situations where the complexity of the first-principles process model is not high, we have shown (Du et al., 2015) that SBMs can be defined as the closed-loop process behavior imposed by an input-output linearizing controller, of the form:

$$\sum_{j=0}^r \beta_j \frac{d^j y}{dt^j} = y^{sp} \quad (14)$$

where r is the system relative order for a single-input, single-output system, and β_j are the time constants of the closed-loop dynamic response. Alternatively, dynamic models of the form (13) can be identified from process operating data using standard system identification techniques. In this case, SBMs take on a specific structure, being in effect a set of multi-input, single-output models, where the inputs are the production-related targets/setpoints defined in the scheduling layer, and the output of each model is a scheduling-relevant process output or state. This structure promotes sparsity and is thus advantageous for optimization calculations (Pattison, Touretzky, Johansson, et al., 2016).

Case study

To demonstrate the feasibility of the proposed approaches, we solve a simple numerical case involving a SISO CSTR and the cyclic production of three products.

The reaction $3R \rightarrow P$ takes place in an isothermal CSTR, while products A, B and C, which are differentiated by their concentration (Table 1) are manufactured in a cyclical mode. The basic dynamic model of the process is shown in Eq. (15).

$$\frac{dx}{dt} = \frac{u}{5000}(1-x) - 2x^3 \quad (15)$$

where u is the feed flow rate (i.e., manipulated variable) and x is the concentration of raw material in the outlet stream (i.e., state variable). In addition to satisfying product demand, an upper limit of 10 hours production time is enforced for each product in the cycle, and the manipulated variable is constrained to $u \in [0, 3000]$. The objective is to maximize hourly profit. We investigate three integrated scheduling and control solution methods, and the results are compared in Table 2. Scheduling solutions for each method are shown in Figure 1.

Scenario 1: following the procedure described in the section ‘‘Simultaneous scheduling and control incorporating mp-MPC’’, the dynamic model of the process is transformed into PWA by solving optimization problems using GAMS/CONOPT. The resulting PWA system and the bounds for state and manipulated variables are used in the MPT toolbox in order to obtain the explicit control solutions. The control solutions are then transformed in explicit constraints and added to constraints from the scheduling problem. The resulting MINLP is solved for production scheduling and control inputs u using GAMS/SBB.

Scenario 2: in this scenario, we follow the procedure described in the section ‘‘Simultaneous scheduling and control incorporating Fast MPC.’’ The dynamic model is discretized and incorporated in the scheduling model. The resulting MINLP is solved for production scheduling and state references using GAMS/SBB. State reference information is sent to the inner control loop, which tracks the performance of the system and can act when facing process disturbances.

Scenario 3: we follow the developments in (Du et al., 2015) and construct an input-output nonlinear controller of the form (14). The controller induces a first order closed-loop response:

$$\frac{dx}{dt} = \frac{1}{\tau_{cl}}(x^{sp} - x) \quad (16)$$

where $\tau_{cl} = 0.25h$ is the closed-loop time constant (in order to account for input saturation during transitions, the corresponding time constant in the SBM used in scheduling calculations was adjusted to 0.35h). Additionally, we approximate the input dynamics with a second order

Hammerstein model of the form (Baldea et al., 2016; Pattison, Touretzky, Johansson, et al., 2016):

$$u = C' Au' + C' Bx^{sp'} \quad (17)$$

with a piecewise constant input transformation: $x^{sp'} = f_{pw}(x^{sp})$.

Models (16) and (17) are embedded in the scheduling problem described above, and the resulting mixed-integer optimization problem is solved sequentially in gPROMS using a rSQP solver with an outer-approximation method to handle the sequence-defining integer variables.

Table 1 – Case Study Steady State Information

Product	u [L/h]	x[mol/L]	Demand rate [kg/h]	Product cost [\$/kg]	Inventory cost [\$/kg]
A	400	0.3032	20	130	1.8
B	1000	0.393	25	125	2
C	2500	0.5	10	120	1.7

Table 2 – Results of integrated problem

Solution method	mp-MPC	Fast MPC	SBMs
Number of variables	153	174	15 differential, 10 algebraic
Number of constraints	540	354	40
CPU Time (s)	83	1	5
Optimal sequence	A-B-C	A-B-C	A-B-C
Cycle time (h)	20.29	18.04	18.37
Revenue (\$)	79646.44	88886.62	94743.61
Raw material cost (\$)	15547.48	16405.73	18772.19
Inventory cost (\$)	6214.34	5468.12	8241.69
Profit (\$)	57884.61	67012.77	67729.72

We notice that integration using Fast MPC provides better results than mp-MPC with a much lower computational time. The superiority of Fast MPC can be explained by aggressive control actions leading to shorter transition times when compared to mp-MPC. Furthermore, Fast MPC is capable of handling large size control problems, and the proposed framework can handle uncertainties in the process operations. Similarly, SBM-based scheduling results in the highest profit of all owing to shorter transition times. The aggressiveness of the controller is reflected in the higher raw material cost for the third scenario (compared to Scenarios 1 and 2), which in this case is reflective of broad and rapid variations in the manipulated input u.

Conclusions and Future Directions

In this work, a simple case study was presented to evaluate the performance of three strategies for the integration of scheduling and control. The frameworks can be adapted to more complex problems involving batch or continuous processes (Touretzky et al., 2016). The results of the simple case study reflect the fact that the execution of production schedules and the economic performance of a process are, indeed, highly dependent on the choice of control system, and provide a strong incentive for investing further efforts in the integration of scheduling and control, both at the fundamental research level and in practical applications.

At the fundamental level, it has become apparent that the integration of scheduling and control requires high-fidelity representations of the process dynamics and associated process control problem. In turn, this calls for the use of nonlinear models capable of accurately describing process behaviors and dynamic transitions. These models are almost invariably high-dimensional, stiff and potentially discontinuous. As a consequence, the computational cost of performing the integrated scheduling/control calculations online and in real-time are quite considerable, and represent one of the main barriers in the deployment of an integrated scheduling/control framework in practical applications. Further efforts are therefore required to develop a systematic and general approach for deriving scheduling-relevant low-order process models. These efforts should be accompanied by progress in fast numerical solution algorithms for mixed integer dynamic optimization problems.

At a higher level, closing the scheduling loop should become a priority. This entails defining and implementing mechanisms that inform rescheduling decisions in the presence of process faults and disturbances that have an impact on schedule execution. These mechanisms should be able to deal with, e.g., plant-model mismatch, equipment faults that do not necessarily entail a complete machine breakdown; moreover, endogenous disturbances, such as changes in feedstock flow rate or composition, and exogenous ones, including changes in market demand and prices of products, utilities or raw materials, should be accounted for.

Closing the scheduling loop should not occur without careful consideration of the stability and feasibility of integrated scheduling/control frameworks. Although the concept of stability has been extensively explored by the control community, it is a new concept for the integrated

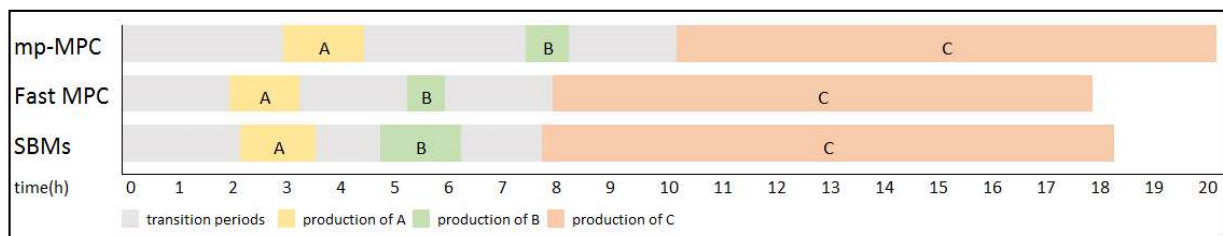


Figure 1. Gantt chart obtained in the three scenarios

scheduling and control scheme and it remains a major challenge (Baldea & Harjunoski, 2014).

Practical challenges will also include data integration across different levels of the decision-making process, in view of the diversity of automation systems and components across different layers of a company. In addition, organizational silos within a company must be broken for an efficient coordination and integration of scheduling and process control. Overall, a closer relationship between industry and academia will be fundamental for proving the business value of an integrated framework and for addressing the remaining challenges in this area.

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