INTEGRATION OF PRODUCTION SCHEDULING AND MODEL PREDICTIVE CONTROL UNDER PROCESS UNCERTAINTIES

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Abstract

In order to achieve optimal operational conditions, the integration of decision-making across different layers of a company and the consideration of uncertain parameters in view of dynamic market conditions are essential. In this study, we propose a framework for the integration of scheduling and control for nonlinear systems under process uncertainties. The framework includes the use of piecewise affine functions (PWA) to handle non-linearities, a robust model predictive control scheme and the use of surrogate models to derive the closed-loop input-output behavior of the dynamic system. We take a preventive approach in handling disturbances at control level. Through a case study, we evaluate the performance of the framework and evaluate the impacts of such disturbances in scheduling solutions.

Keywords

Robust model predictive control, production scheduling, integrated scheduling and control, surrogate-based optimization

Introduction

The problem of integrating production scheduling and process control has gained increasing attention by academia and industrial communities as research shows the possibility of improving performance when the decision making processes across all the layers of the chemical supply chain are addressed simultaneously (Grossmann, 2005). Furthermore, such integration seems natural given the closer relation between scheduling and control problems, and the extensive exchange of information required for the solution of both problems.

The most intuitive approach for the integration of scheduling and control involves the incorporation of the dynamic behavior of the process to the scheduling problem and developing techniques to solve the resulting mixed integer dynamic optimization (MIDO) problem. These approaches, however, face considerable challenges associated to the use of high-fidelity representations of the process dynamics and the complexity, nonlinearities and discontinuities that this brings to the scheduling problem. The computational cost of performing the integrated scheduling/control calculations online and in real-time represent one of the main barriers in the deployment of an integrated scheduling and control framework in practical applications. Furthermore, most of the frameworks proposed so far neglect the dynamic market conditions to which process industries are subject, and fail to address the effects of uncertainties in process operation.

Uncertainties can be associated to exogenous and endogenous factors, and can be effectively handled by the scheduling and control problems depending on its source. Disturbances such as flow and rate temperature variations, stream quality fluctuations, and dynamic model mismatches are associated to the control problem, while disturbances related to product demands, prices, processing times and equipment availability affect mainly scheduling solutions. Furthermore, based on the availability of information, uncertainties can be described by probability functions or by upper and lower bounds, and approaches for dealing with uncertainties can be classified as preventive or reactive (Li & Ierapetritou, 2008). In reactive approaches, solutions for scheduling and control problems are based on nominal models, and are updated in response to the occurrence of uncertainties. Preventive approaches, on the other hand, incorporate the model of uncertainty in the scheduling and control formulations and generate robust solutions prior to the occurrence of a disturbance.

In this work, we focus our attention in disturbances at the control level and propose a preventive framework for the integration of production scheduling and model predictive control (MPC) for nonlinear systems under process uncertainties. Compared to recent works in the integration of scheduling and MPC (Baldea et al., 2015; Zhuge & Ierapetritou, 2015), our main contributions are: i) the use of a robust model predictive control in the integrated

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framework; ii) a comparison between integrated frameworks using deterministic and robust control strategies; and iii) the use of surrogate based techniques to derive closed-loop input-output relationships of systems controlled by different MPC schemes. The models are added as constraints on the scheduling problem, resulting in a mixed integer nonlinear program (MINLP) formulation.

The general algorithm for the integration of scheduling and control is presented in the next section. The first step is to approximate the nonlinear dynamics of the system using a piecewise affine (PWA) model identification technique described in the section “PWA for nonlinear MPC”. Then we propose to handle uncertainties at control level by introducing a robust model predictive control scheme in section "Robust model predictive control". Surrogate models are built to approximate the control actions and closed loop behavior of the dynamic system, and the integration of robust MPC and production scheduling is achieved following the formulation presented in section "Scheduling problem formulation". A case study illustrates the performance of the framework, followed by discussions and conclusions.

Framework for integration of scheduling and robust control using surrogate models

The main components of the framework for the integration of scheduling and robust MPC are described in the following sections and are shown in Figure 1. We first approximate the nonlinear dynamic behavior of the system with piecewise affine functions. Then, a robust control scheme based on model predictive control is built, so uncertainties such as model mismatch and internal disturbances can be appropriately handled. The third step is to use surrogate models to approximate the closed-loop input-output relationships, control actions during transition and transition times imposed by the robust control. The models are incorporated to the scheduling formulation as constraints, and the scheduling problem is solved for state references and production sequences. This information is then transmitted to the robust control, which tracks the state references online. If some disturbance affects the system leading the state values away from its quality bounds, re-scheduling is triggered and a new scheduling solution is implemented.

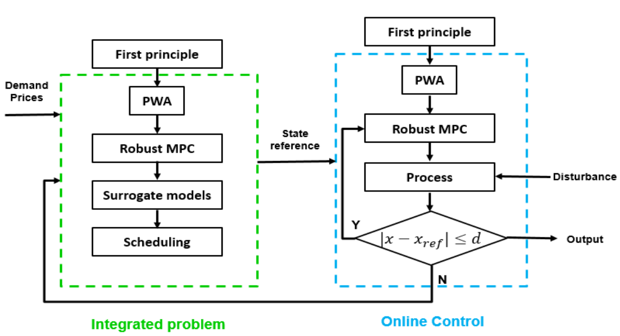

Figure 1. Algorithm for the integration of scheduling and robust MPC

PWA for nonlinear MPC

PWA systems have shown to be an effective approach in dealing with nonlinear systems. The basic idea of PWA system is that the nonlinear dynamics can be approximated by a collection of distinct linear (or affine) dynamic approximations with associated regions of validity. Compared to standard linear models, PWA composes a group of linear models and therefore it is capable to address the process dynamics at the entire state domain. Therefore, PWA models eliminate the nonlinearity while retaining high approximation accuracy.

If the original nonlinear dynamic model of the system is known, the piecewise affine functions can be identified using optimization based identification techniques. We follow the technique presented by Dias et al. (2016), which can be summarized as follows:

For one-dimensional functions, valid regions VR and PWA functions $\hat{f}$ are defined as:

$$VR_i = \{x | x_{int,i-1} \leq x \leq x_{int,i}\}, i \in I = \{1,2,\ldots,N_i\} \tag{1}$$

$$\hat{f}(x) = a_i x + b_i, if\ (x) \in VR_i \tag{2}$$

The domain of the original nonlinear function $f(x)$ is partitioned in N_i regions, generating N_i intermediate points $x_{int,i}$. Each valid region can then be defined by the interval between two consecutive intermediate points. The PWA function associated to each valid region assumes the form of Eq. (2). Coefficients a_i and b_i can be determined by solving the optimization problem given by Eq. (3), which includes constraints to enforce continuity at the intersection points (Eq. 4). Note that if the continuity at the intersection points is established, then the continuity at the whole domain of $f(x)$ is established as well.

$$\min_{x,a_i,b_i} \sum_i \left(\hat{f}(x_{int,i}) - f(x_{int,i})\right)^2 \tag{3}$$

$$s.t.\ a_i x_{int,i} + b_i = a_{i+1} x_{int,i} + b_i \tag{4}$$

For multi-dimensional functions that can be classified as separable functions, i.e., functions that can be written as a sum of functions of single variables, PWA approximations can be obtained by applying one-dimensional approximations as explained above for each term of the function. For non-separable equations, we follow the procedures suggested in Szucs et al. (2012) in converting non-separable functions into the separable form, summarized as follows:

Procedure 1: if the function $f(x_1, x_2, \ldots, x_n)$ is in form of a product, i.e. $f(x_1, x_2, \ldots, x_n) = f(x_1)f(x_2)\ldots f(x_n)$, then introduce new variables to transform the product into a separable function. For example, for a function f given by $f = x_1 x_2$, let $y_1 = x_1 + x_2$ and $y_2 = x_1 - x_2$, then $x_1 x_2 = (y_1^2 - y_2^2)/4$, and the function f transformed to a separable form is $f = (y_1^2 - y_2^2)/4$.

Procedure 2: if the function $f(x)$ can be written in the form of Eq. (5), first obtain the PWA approximation of the inner function, then define $w = f_{in}(x)$ and approximate the function $f_{out}(w)$.

$$f(x) = f_{out}\big(f_{in}(x)\big) \quad (5)$$

A n-dimensional separable function will have the form: $f = f^1(x^1) + f^2(x^2) + \cdots + f^n(x^n)$. PWA functions can be defined for each one-dimensional function $f^k, k = 1,2, \dots n$, and the PWA function for f can be written as $\hat{f} = \hat{f}^1 + \hat{f}^2 + \cdots \hat{f}^n$.

The variables in a dynamic model of a system will include the state variables x, control variables u and uncertain parameters δ. A PWA for a system with one state variable, one control input and one uncertain parameter will have the form:

$$x_{k+1} = A_i x_k + B_i u_k + C_i \delta + D_i, if\ (x, u, \delta) \in VR_i \quad (6)$$

Robust Model Predictive Control

In process operations, disturbances such as flow and rate temperature variations, stream quality fluctuations and model mismatch (including, for example, mass/heat transfer coefficients and kinetic constants) must be handled by an appropriate control. In the fields of advanced process control and, more specifically, model predictive control, control schemes for uncertain systems arise specially in the form of robust MPC. Robust MPC was first proposed by Campo and Morari (1987), who considered the possibility of model mismatch and assumed that the system behavior could be described by a set of linear time invariant (LTI) models instead of a single LTI. They proposed to minimize the worst-case tracking error for the family of linear plants, and showed how to recast the resulting minimax optimization problem as a linear program. This approach was further extended by Allwright and Papavasiliou (1992) and Zheng and Morari (1993), and can be classified as open-loop robust MPC formulation. Open-loop MPC solves optimization problems in which the decision variable is a sequence of control actions, and ignores the fact that the controller will react to the uncertainty in the next steps, which may lead to infeasibilities and conservative solutions. Therefore, closed-loop robust MPC was proposed by Kothare et al. (1996) and (Lee & Yu, 1997), and the optimization problem was solved for a control policy, which is a sequence of control laws, overcoming the drawbacks of open-loop robust MPC.

More recently, tube-based MPC has been presented by Mayne et al. (2005). In tube based control, an ancillary controller that constraints deviations of the state of the uncertain system from the nominal trajectory is determined. Recent advances in tube model predictive control regarding the calculation of ancillary controller are presented by Rakovic et al. (2012) and Yu et al. (2013).

The purpose of this paper is to evaluate the benefits of using a preventive control scheme and the impacts of disturbances at the control level in the scheduling solutions. Therefore, we propose a simple open-loop robust control strategy for nonlinear systems described by a set of PWA functions, summarized as follows:

Step 1: Set initial states and initial manipulated variables x^0, u^0

Step 2: Locate corresponding LTI for current states.

If $x \in \Omega_i = \{x: V_i x \leq W_i\}$, $i \in S_i = \{1,2, \dots, N_i\}$, then select $LTI^i: x_{k+1} = A_i x_k + B_i u_k + C_i \delta + D_i$

Step 3: Minimize the worst-case tracking error by solving the robust MPC problem for PWA systems (Eq. 7), where a dynamic reference $\bar{x}_{k+k_p}$ is tracked.

$$\min_{u_k} \max_{\delta} \sum_{k_p=1}^{N-1} \left(\left\| x_{k+k_p} - \bar{x}_{k+k_p} \right\|^{Q_{k_p}} + \left\| u_{k+k_p-1} - \bar{u}_{k+k_{p-1}} \right\|^{R_{k_p}} \right) + \| x_{k+N} - \bar{x}_{k+N} \|^{Q_N} \quad (7)$$

$$s.t. \begin{cases} x_k = x^0 \\ x_{k+k_p} = A_i x_{k+k_p-1} + B_i u_{k+k_p-1} + C_i \delta_{k+k_p-1} + D_i, \\ x_{min} \leq x_{k+k_p} \leq x_{max}, \\ u_{min} \leq u_{k+k_p} \leq u_{max}, \end{cases}$$

where N is the time horizon and Q and R are the performance weights.

Step 4: Evaluate state transfer $x_{k+1} = f(x_k, u_k)$

Step 5: $k = k + 1$, go to step 2.

Surrogate modeling

Scheduling and control are naturally related problems, and process operations at scheduling and control levels require data exchange between them. For example, scheduling transfer decisions such as batch sizes, start times and state references to the control level, while control provides transition times and dynamic behavior of the system to the scheduling level. Therefore, the simultaneous solution of scheduling and control problems can lead to decisions that are overall optimal. Attempts to integrate scheduling and control include the use of the dynamic models of the system as constraints in the scheduling problem (Flores-Tlacuahuac & Grossmann, 2006), use of explicit control laws derived through multi-parametric MPC (Zhuge & Ierapetritou, 2014), and the use of time-scale bridging models (Du et al., 2015).

In this work, we propose to use surrogate models to approximate the closed-loop input-output dynamics of the process, the transition times and the average value of the control actions taken during transitions, which will be further incorporated as constraints in the scheduling problem. Many fields in engineering have successfully used surrogate models to solve optimization problems characterized by partial or total lack of analytical equations describing the constraints and objective of the problem. In particular, surrogate modeling techniques are of great interest for engineering design when high fidelity and expensive analysis codes are used, such as the fields of computational fluid dynamic models and large-scale integrated flow sheet models.

The proposed framework for building surrogate models can properly handle problems associated to the different time horizons in which scheduling and control problems are defined, and provides a simple way to derive an explicit expression to approximate the closed-loop behavior of a process imposed by a general control. We consider a system with n state variables and m manipulated variables, and consider the problem of scheduling in a multiproduct plant. The framework follows common basic steps and can be summarized as follows:

Step 1: Determine the sample points in the design space using design of experiments. In particular, Latin Hypercube Sampling is used with $10d+1$ samples, where $d=n+m$ is the number of dimensions. The variables of the dynamic problem are the initial values of states x^0 and control inputs u^0.

Step 2: Run simulations to collect the observed results at each sample point. For each simulation, the input data are the initial conditions of the system defined by step 1 and steady state information for the desired product. The outputs of the simulations are the average control actions during transitions, the transition times, and the values of the future states x_{k+1}.

Step 3: Build three surrogate models for each product p using kriging models. The first surrogate model predicts the average value of control actions during transitions, $\bar{u}$. The second surrogate model predicts the transition times θ. The third surrogate predicts future states x_{k+1}, where the time length of k is pre-defined by the user.

Kriging was originally developed in geostatistics by Krige (1951), and it was later applied to both deterministic and stochastic simulation models for developing input-output relationships. For the derivation of Kriging, the output of a deterministic computer experiment is treated as a realization of a random function (Eq. 8). The function is defined as the sum of a global trend function, which here will be taken as a constant β_0, and a Gaussian random function $Z(x)$. Z denotes a statitionary random process with zero mean, variance σ^2 and nonzero covariance (Eq. 9), where $R(x_i,x_j)$ is the correlation function. The kriging predictor for a point x^* can then be written as Eq. (10), in which $\boldsymbol{R}$ is defined as the $(n\times n)$ matrix where the (i,j) element is the correlation between $Z(x_i)$ and $Z(x_j)$, and r is defined as the correlation vector between $Z(x^*)$ and $Z(x_i)$, for $i=1,\ldots,d$. The generalized least square estimation of β_0 is given by Eq. (11).

$$y(x)=\beta_0+Z(x) \tag{8}$$

$$Corr\left[Z(x_i),Z(x_j)\right]=\sigma^2R(x_i,x_j) \tag{9}$$

$$\hat{y}(x^*)=\beta_0+r^T(x^*)\boldsymbol{R}^{-1}(y_s-\beta_0\mathbf{1}) \tag{10}$$

$$\beta_0=(1^T\boldsymbol{R}^{-1}\mathbf{1})^{-1}1^T\boldsymbol{R}^{-1}y_s \tag{11}$$

The surrogate models built in this step can be written in a general form as given by Eqs. (12-14).

$$\bar{u}_p=F_p(x^0,u^0) \tag{12}$$

$$\theta_p=G_p(x^0) \tag{13}$$

$$x_{k+1,p}=H_p(x^0,u^0) \tag{14}$$

Scheduling problem formulation

In this work, the problem of continuous cyclic production is addressed, and scheduling constraints are adapted from the work of Flores-Tlacuahuac and Grossmann (2006). Constraints at control level include the surrogate models predicting the transition times and the control actions during transitions. These models, given by Eq. (12) and (13), are valid when product p is produced in slot s, and this implicit requirement is transformed into explicit constraints (Eqs.15-18).

$$\bar{u}_s\geq F_p(x^0,u^0)-M(1-y_{p,s}) \tag{15}$$

$$\bar{u}_s\leq F_p(x^0,u^0)+M(1-y_{p,s}) \tag{16}$$

$$\theta_s\geq G_p(x^0)-M(1-y_{p,s}) \tag{17}$$

$$\theta_s\leq G_p(x^0)+M(1-y_{p,s}) \tag{18}$$

where $y_{p,s}$ is 1 if product p is produced in slot s, and (x^0,u^0) are the steady state conditions of the previous slot, calculated with the use of linking constraints as presented in the work of Zhuge and Ierapetritou (2015). The objective function of the problem is the maximization of total profit Φ, which is given by Eq. 19.

$$\Phi=\sum_{p=1}^{N_p}P_pW_p-\left(\sum_{s=1}^{N_s}P_ru_s^n\Theta_s+\sum_{s=1}^{N_s}P_r\bar{u}_s\theta_s\right) \quad (19$$

where N_p is the number of products, P_p is the price of product p, W_p is the amount of product p produced in a cycle, N_s is the number of slots, u_s^n is the nominal value of the control variable in slot s, P_r is the cost of raw material and Θ_s is the production time.

The scheduling problem is solved for the production sequences. Once the sequences are defined, the state values throughout transitions can be calculated using Eq. 14. Such values are used as references in the online control loop.

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 four products.

The reaction 3R→ P takes place in an isothermal CSTR, while products A, B, C and D, which are differentiated by their concentration (Table 1) are manufactured in a cyclic mode. The basic dynamic model of the process is shown in Eq. (26).

$$\frac{dx}{dt}=\frac{u}{5000}(1-x)-kx^3 \tag{26}$$

where u is the feed flow rate (i.e., manipulated variable) and x is the concentration of raw material in the outflow (i.e., state variable). In addition to satisfying product demand, an upper limit of 144 hours is enforced for the production cycle, and the manipulated variable is constrained to $u\in[0,3000]$. The objective is to maximize hourly profit.

Table 1 – Case Study Steady State Information

Product	u [L/h]	x[mol/L]	Demand rate [kg]	Product cost [$/kg]
A	100	0.2	5500	30
B	400	0.3032	8000	20
C	1000	0.393	10000	15
D	2500	0.5	14000	10

We build two scenarios to solve the scheduling problem: in the first one we use a deterministic MPC while the second one uses the robust MPC for building surrogate models and for online control. We assume the kinetic constant k is uncertain. In the first scenario, $k = 2\ lt^2 mol^{-1} h^{-1}$, while in the second scenario k is bounded and in the form $k = [2{,}2.3]\ lt^2 mol^{-1} h^{-1}$. Following our framework, we built a PWA system to represent the dynamic model assuming that x, u and k are the variables. The control schemes are proposed, differing only on step 3 on the control algorithm, where the first scenario uses the deterministic MPC instead of the robust one. Trough simulations the surrogate models are built, and the scheduling problem is solved using GAMS/SBB. The results are presented in table 2.

Table 2 – Results of integrated problem

	Integration using Deterministic MPC	Integration using Robust MPC
Number of variables	138	138
Number of constraints	82	82
CPU Time (s)	4	4
Optimal sequence	A-D-C-B	A-C-D-B
Transition times	7.62–2–1.95-3.24	8.02-3.24-1.67-1.33
Amount (10^3kg)	5.5-14-12-8.21	5.5-8-10.13-14
Revenue ($/hr)	4509.08	4284.74
Raw material cost ($/hr)	2619.31	2470.92
Profit ($/hr)	1889.77	1813.82

We notice that the framework using deterministic MPC provides slightly better profit than robust MPC. This is a result of the different control actions taken during transitions and production times. However, the advantages of the solutions from deterministic MPC are specific to this example and to the given parameters. Furthermore, robust MPC has the advantage of effectively handling uncertainties and guaranteeing feasible solutions in the presence of uncertainties, as it is shown in the simulations below.

We first assume that no disturbances affect the system, and therefore the value of the kinetic constant is kept at $2\ lt^2 mol^{-1} h^{-1}$ throughout the whole simulation. We simulate the behavior of robust and nominal control and the results are shown in Figure 2.

Next, we assume that the uncertain parameter k assumes its nominal value throughout most of the simulation period, with the exception of times t=100h to t=110h, when $k = 2.3\ lt^2 mol^{-1} h^{-1}$.

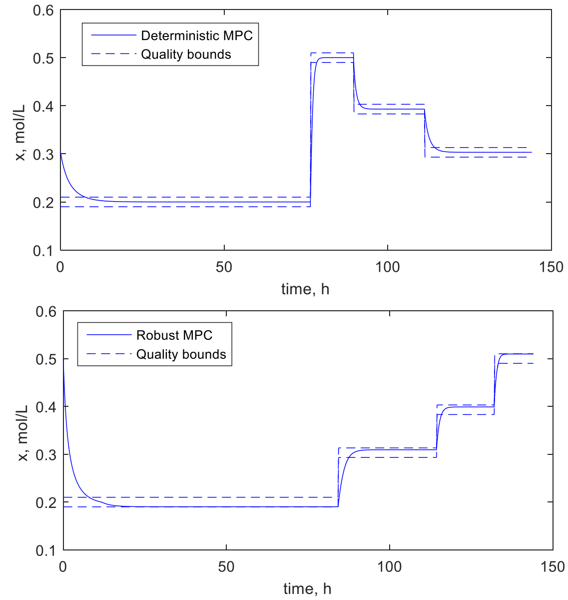

Figure 2. Simulations for deterministic and robust control when no disturbances affect the process

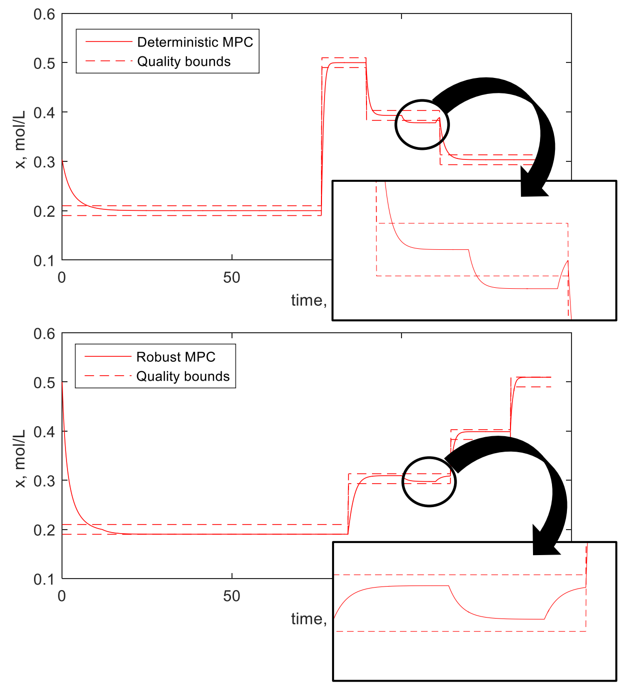

Figure 3. Simulations for regular and robust control in a system affected by disturbances from times t=100h to t=110h

While the robust control can effectively handle the uncertainties that affect the system, the nominal control cannot. For 9.33 hours, the production of C is affected, period in which the product does not meet the quality requirements and therefore we assume it cannot be commercialized. Consequently, the demand of C in the given time horizon will not be satisfied and the hourly profit decays to $1299.65. In this case, re-scheduling will be triggered, however the problem will be infeasible, since the demands of C and D will cannot be satisfied in the remaining time. The preventive scenario, on the other hand, is able to handle the disturbances and ensures that the product specifications are met during the whole time horizon.

The computational cost of the integrated problem can be evaluated by the number of simulation calls in the surrogate building step and CPU time of scheduling solutions. For the second scenario of this problem, $4 * (10n + 1)$ or 84 simulation calls were done, and the CPU time for scheduling solutions was 4 seconds. Calculations were performed using a PC of 2.40GHz/16GB RAM.

Conclusions and Future Directions

In this study, we propose a novel framework for the integration of scheduling and control. This framework aims to simultaneously consider the scheduling and control objectives and is capable of handling disturbances to the dynamic system in a preventive manner, avoiding infeasibilities and reducing calls for re-scheduling. The framework includes the use of a robust model predictive control scheme and the use of surrogate models to predict the closed-loop input-output behavior of the system, and can be extended to a wide variety of process in which different control strategies are applied. A simple case study was presented to demonstrate the performance of the framework and its advantages when compared to the integration of scheduling and deterministic control.

The results of the case study show a superiority of the deterministic MPC framework in the nominal scenario, and superiority of the robust MPC framework in a scenario subject to disturbances. Although these results cannot be generalized, they provide some useful insights. Robust MPC is capable of handling disturbances in a more effective way when compared to deterministic MPC. Therefore, in a scenario where the process is subject to disturbances in the control level, the integration of scheduling and robust MPC is more likely to provide feasible solutions, and may guarantee higher profits if disturbances are frequent.

Future challenges include addressing higher dimensional problems, as well as integrating scheduling and control while considering uncertainties in both scheduling and control levels.

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