12th IFAC International Symposium on
Advanced Control of Chemical Processes
July 14-17, 2024. Toronto, Canada

Integrated scheduling and control with closed-loop prediction ⋆

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Abstract: Dynamic market conditions as a consequence of increased globalization, coupled with fluctuations in electricity prices brought about by the deregulation of energy markets, require process manufacturing plants to operate in a responsive manner in order to remain competitive. In particular, the quasi steady-state assumption that is typically applied in optimal scheduling does not hold in a highly dynamic operating environment, where the dynamics of transitions have an increasingly significant impact. This has led to a research thrust on the integration of scheduling and control. In this paper, we provide an overview of this topic, highlighting assumptions and formulations related to the plant control system. We then focus on a class of 'controller aware' scheduling formulations, in which the predicted closed-loop response of the plant under the action of the plant control system is taken into account. A case study illustrating key concepts is presented.

Keywords: Scheduling and control, closed-loop prediction, dynamic real-time optimization

1. INTRODUCTION

Traditionally, chemical manufacturers follow a hierarchical decision-making architecture, an example of which is shown in Fig. 1. The downwards arrows indicate production targets while the upward arrows indicate feedback information. In some paradigms, the real-time optimization (RTO) layer may be absent, or be replaced by a dynamic real-time optimization (DRTO) problem. Steady-state models have typically been used in the scheduling layer. However, increasingly volatile market conditions, shaped by the deregulation of the electricity prices and growing participation of intermittent energy sources in the power grid, require set-point transitions to be performed more often to efficiently respond to fluctuations in product demand and raw material costs, for example. In this new operating paradigm, the process dynamics become relevant to the scheduling decisions, and should be accounted for in the scheduling layer (Baldea and Harjunkoski, 2014) to improve economic performance. This has motivated efforts for the integration of scheduling and control.

The integration of scheduling and control is often advocated as a pathway to improve the response time and flexibility of production processes (Caspari et al., 2020). One of the reasons is that providing the scheduling problem with more detailed information about the process dynamics has the potential to reduce plant-model mismatch, increasing the chances of a feasible schedule with achievable production targets being generated. Another reason is that the integrated scheduling and control problem is solved more often than the traditional scheduling problem, increasing the feedback frequency. Therefore, any disturbances to the schedule are perceived (and dealt with) faster than in the traditional approach.

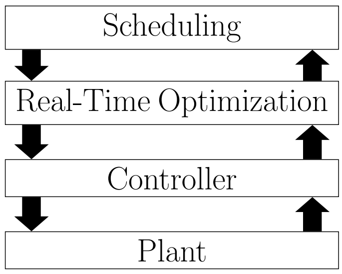

Fig. 1. Typical decision-making hierarchy in the chemical industry.

In the next section we discuss various paradigms for the integration of scheduling and control. In Section 3, we present an overview of integrated scheduling and control with closed-loop prediction. That is followed by an illustrative case study, and conclusion.

2. INTEGRATION OF SCHEDULING AND CONTROL

Various paradigms for the integration of scheduling and control have been proposed in the literature. The two more prominent ones are the single-level and hierarchical approaches. In both of them, the typical steady-state based scheduling model gives way to a dynamic process model. However, in the hierarchical paradigm, some studies propose to virtually account for the control dynamics in addition to the process dynamics. These are deemed 'controller aware' formulations (Flores-Cerrillo et al., 2024) because

⋆ Financial support from Research Excellence (ORF-RE) Award RE09-058 and McMaster Advanced Control Consortium (MACC)

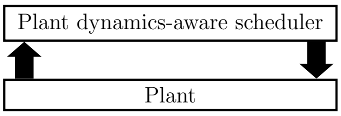

Fig. 2. Single-level paradigm for the integration of scheduling and control.

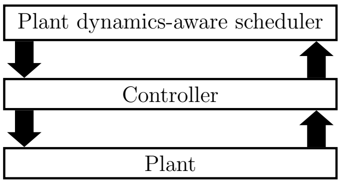

Fig. 3. Hierarchical paradigm for the integration of scheduling and control.

they predict the closed-loop response of the process. That is, the process response under the feedback control action.

In the single-level approach, the computed scheduling decisions and input values are directly applied to the plant without necessitating a controller. With reference to the diagram in Fig. 1, this means integrating the scheduling, real-time optimization and controller layers into a single layer as presented in Fig. 2. The single-level approach can also be considered as an extension of economic model predictive control (EMPC) (Ellis and Christofides, 2014) to scheduling decisions. In the hierarchical paradigm, the integrated scheduling and control problem is solved at the RTO level to provide set-points to the control system. The hierarchical paradigm of Fig. 3 captures integration of the scheduling and real-time optimization layers in Fig. 1, with or without a virtual integration of the control system.

Single-level paradigm

Several studies in the literature follow the single-level paradigm. However, not all of them consider a closed-loop implementation of the optimal decisions, focusing instead on the development of the integrated scheduling and control formulation. The formulation developed in Flores-Tlacuahuac and Grossmann (2006) computes the optimal cyclic schedule of multiproduct CSTRs. The transition times have to be determined iteratively as part of the solution of the integrated problem in order to obtain an acceptable trajectory. Zhuge and Ierapetritou (2012) develop a similar formulation but, in addition, propose a strategy for closed-implementation that consists of re-computing the optimal control and scheduling decisions when the deviation between the predicted and observed state trajectories exceeds a specified threshold. Simkoff and Baldea (2020) propose a stochastic integrated and control formulation for a chlor-alkali process. They consider uncertainty in electricity demand and price. Chu and You (2013b) develop a two-stage stochastic formulation for batch processes that accounts for model uncertainty. A scheduling and control formulation for hydropower systems subjected to electricity price uncertainty is presented in Mathur et al. (2021).

The integration of scheduling and control typically yields a mixed-integer nonlinear programming (MINLP) problem due to the nonlinear dynamic process model and the discrete scheduling decisions. A number of studies have proposed methods to reduce the integrated problem complexity and solution time. Andres-Martinez and Ricardez-Sandoval (2021) utilize concepts of switched systems to convert their MINLP formulation to a nonlinear programming (NLP) problem. Alternatively, Chu and You (2013a,b) and Nie et al. (2015) propose methods based on generalized Benders decomposition to reduce the solution time.

Hierarchical paradigm

A disadvantage of the single-level paradigm is that it requires the solution of a large scale dynamic optimization problem at every sampling-time. Failure to solve this problem could potentially lead to reliability and safety issues. This is one of the main motivations for the hierarchical paradigm, which keeps the existing controller layer in chemical manufacturing industries intact. Therefore, even if the integrated problem fails to be solved, set-point trajectories could be manually assigned to the plant controller to maintain safe process operation.

As previously mentioned, there are two main variations within the hierarchical paradigm. The first one utilizes an open-loop representation of the process dynamics. The second one accounts for the closed-loop process dynamics. That is, it models the control dynamics in addition to the plant dynamics, and is thus *controller aware* (Flores-Cerrillo et al., 2024). Control-aware formulations compute optimal set-point trajectories for the control system, while in open-loop formulations, the set-point trajectories have to be extracted from the predicted state, output and input trajectories in some fashion. We discuss control-aware formulations in more detail in Section 3.

Open-loop formulations for the integrated scheduling and control problem are proposed in Andrés-Martínez and Ricardez-Sandoval (2022) and Zhuge and Ierapetritou (2015). They typically have lower computational complexity than their closed-loop counterpart since they neglect the lower-level control dynamics. However, for the same reason, open-loop formulations have inherent plant-model mismatch, even under perfect knowledge of the plant model.

3. CONTROL-AWARE SCHEDULING FORMULATIONS

Control-aware scheduling formulations are referred to as closed-loop formulations because they predict the closed-loop process dynamics. Therefore, they eliminate the plant-model mismatch resulting from neglecting the impact of the control system on the plant dynamics that is inherent in the open-loop prediction counterpart. Additionally, knowledge of the control systems allows control-aware formulations to compute feasible and reachable set-point trajectories for the lower-level controller. Scheduling decisions such as production sequencing can be communicated to the plant exclusively through these set-point trajectories.

Several control-aware formulations for the integrated scheduling and control problem have been proposed in the literature. These include formulations tailored to processes controlled by linear model predictive control (LPMC)

(Dias et al., 2018; Remigio and Swartz, 2020; Simkoff and Baldea, 2019; Burnak et al., 2018; Zhuge and Ierapetritou, 2014; Dering and Swartz, 2023a), input-output linearizing controllers (Du et al., 2015; Kelley et al., 2018), and PI controllers (Dering and Swartz, 2023b; Chu and You, 2012).

The LMPC aware formulations differ on several fronts, including the strategy utilized to account for the control action and solve the integrated problem. Because LMPC is itself an optimization problem, accounting for its action within an integrated scheduling and control formulation leads to a multilevel dynamic optimization problem for which a specialized solution strategy is required.

Dias et al. (2018) develop a state-space data-driven model for an air separation unit. The input actions applied to the data-driven model are computed via solution of a LMPC problem. They utilize a simulation-based optimization strategy to solve the resulting multilevel problem. The optimization is carried out by iteration between an optimization calculation in which decision variables are adjusted, and closed-loop simulation that provides sensitivity information to the optimizer. This process continues until a convergence criterion is met. The optimal set-point trajectories are tracked online by the lower-level LMPC controller to compute the input values applied to the plant.

Remigio and Swartz (2020); Dering and Swartz (2022) and Simkoff and Baldea (2019) take advantage of the convexity properties of the LMPC problem, and replace the embedded LMPC problems within their integrated scheduling and control formulation by the equivalent first-order Karush-Kunh-Tucker (KKT) conditions. This effectively reduces the multilevel optimization problem to a single-level mathematical problem with complementarity constraints (MPCC). Simkoff and Baldea (2019) utilize a nonlinear model representation of the process in their integrated formulation, and use complementarity conditions to model discrete scheduling decisions. A penalization approach that consists of penalizing the complementarity constraints in the objective function is used to solve the integrated problem. Real-time execution of the scheduling and control problem is not considered, and the scheme is applied to single product plants that do not require sequencing decisions. In Remigio and Swartz (2020) and Dering and Swartz (2022), the integrated problem is solved online at predefined time intervals to compute set-point trajectories for the lower-level controller. They consider mutiproduct processes, and the production sequencing is communicated to the plant exclusively through the set-point trajectories assigned to the LMPC controller. While a discrete-time state-space approximation of the nonlinear plant model is utilized in the formulation in Remigio and Swartz (2020), Dering and Swartz (2022) use piecewise linear segments to approximate the nonlinear plant model. In both studies, binary variables are introduced to reformulate the LMPC-KKT conditions as mixed-integer linear constraints, and a disturbance estimate is used to address plant-model mismatch.

As previously mentioned, control-aware scheduling formulations are computationally more expensive than their open-loop counterpart. This has motivated the development of strategies to reduce their computational burden. Zhuge and Ierapetritou (2014) use multiparametric programming to obtain an explicit solution for the LMPC problem. This solution is then utilized within their integrated scheduling and control framework to compute the input actions applied to the process model. Burnak et al. (2018) go a step further and obtain offline solution maps for the control-aware scheduling problem itself, reducing its online solution time to a look-up table and a function evaluation. An alternative strategy is adopted in Dering and Swartz (2022). They use an unconstrained LMPC formulation coupled with an input clipping mechanism as a surrogate for its constrained counterpart. Since the unconstrained LMPC problem has an explicit solution, the solution time is significantly reduced.

Given the market volatility and inherent processes uncertainties, a robust control-aware formulation could prove beneficial. There are at least two strategies to deal with uncertainty within the context of the integration of scheduling and control. One is via feedback and periodic solution of a deterministic problem. The other is to explicitly account for uncertainty in the problem formulation using stochastic programming or robust optimization methods. In the latter, the integrated problem can also be solved periodically to incorporate feedback information. An interesting discussion of the impacts of the re-scheduling frequency, uncertainty and scheduling horizon on the quality of the executed schedule is provided in Gupta et al. (2016); Gupta and Maravelias (2016) in the context of state task network (STN) formulations. A control-aware formulation that explicitly accounts for uncertainty in product demand is proposed in Dering and Swartz (2022), and later extended to account for uncertainty in cost and model parameters in Dering and Swartz (2023b).

4. CASE STUDY

In this section, we present an illustrative case study of a nonlinear plant operated under a control-aware scheduling formulation. A schematic representation of the decision-making configuration is presented in Fig. 4. At the DRTO level, we solve the control-aware scheduling problem to compute the set-points trajectories y_{j*}^{SP} tracked by the lower-level linear MPC. The MPC controller computes the input values $u_{j*,0}$ applied to the plant. Output y_{j*}^{m} and inventory $I_{j*,g}$ measurements are provided as feedback information from the plant to the upper layers. The DRTO problem is solved periodically to account for real-time market and plant information.

4.1 Plant

The plant is represented by a nonlinear CSTR model adapted from Ellis and Christofides (2014) where a reaction $A \rightarrow B$ takes place:

$$\frac{dT}{dt} = \frac{F}{V_R}(T_0 - T) - \frac{\Delta H k_0}{\rho c_p} e^{-E/RT} C_A + \frac{Q}{\rho c_p V_R} \quad (1)$$

$$\frac{dC_A}{dt} = \frac{F}{V_R}(C_{A0} - C_A) - k_0 e^{-E/RT} C_A \quad (2)$$

The inputs are the inlet concentration C_{A0} and heat input Q to the reactor. The outputs are the concentration C_A and temperature T in the reactor. This process produces three product grades, A, B and C. More details about

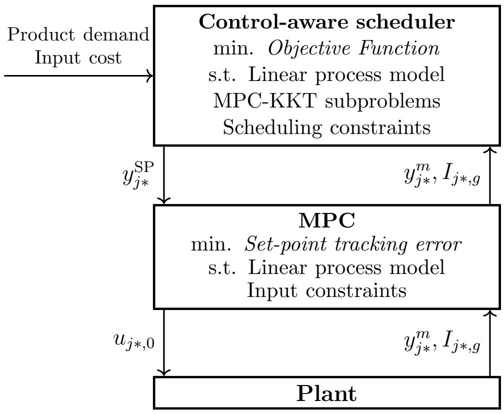

Fig. 4. Schematic representation of case-study framework.

this process, including the model parameter values, can be found in Dering and Swartz (2023b).

4.2 Model predictive controller (MPC)

The lower-level MPC problem is formulated as:

$$\min_{u_{j,k}} \quad \sum_{k=1}^{P} \left(y_{j,k} - y_j^{\mathrm{SP}}\right)^T Q \left(y_{j,k} - y_j^{\mathrm{SP}}\right) + \sum_{k=0}^{M-1} \left(\Delta u_{j,k}\right)^T R \left(\Delta u_{j,k}\right) \tag{3}$$

subject to:

$$x_{j,k+1} = Ax_{j,k} + Bu_{j,k} \qquad \forall k \in \mathcal{J}_0^{M-1} \tag{4}$$

$$x_{j,k+1} = Ax_{j,k} + Bu_{j,M-1} \qquad \forall k \in \mathcal{J}_M^{P-1} \tag{5}$$

$$y_{j,k,i} = Cx_{j,k} + d_j \qquad \forall k \in \mathcal{J}_1^{P} \tag{6}$$

$$\Delta u_{j,k} = u_{j,k} - u_{j,k-1} \qquad \forall k \in \mathcal{J}_0^{M-1} \tag{7}$$

$$u_{\min} \leq u_{j,k} \leq u_{\max} \qquad \forall k \in \mathcal{J}_0^{M-1} \tag{8}$$

where $Q > 0$, and $R \geq 0$ are diagonal weighting matrices. A, B and C are state-space matrices. M and P are the control and prediction horizon, respectively. We define $\mathcal{J}_a^b = \{i | a \leq i \leq b, i \in \mathcal{Z}\}$ as the set of discrete time-steps. The subscript j indicates the simulation time-step in the closed-loop simulation studies, and the DRTO time-step in the control-aware scheduling formulation discussed in next section. $y_{j,k} \in \mathcal{R}^{n_y}$, $u_{j,k} \in \mathcal{R}^{n_u}$, and $x_{j,k} \in \mathcal{R}^{n_x}$ are output, input and state vectors, respectively. d_j is a disturbance estimate given by $d_j = y_j^m - Cx_{j-1,1}$, where y_j^m is the vector of output measurements. y_j^{SP} is a vector of output set-points computed via the solution of the control-aware scheduler problem in the next section.

4.3 Control-aware scheduler

In this section, we present an overview of the control-aware scheduling formulation used in this case study. We refer the reader to Dering and Swartz (2023a) for more details.

Process model: We use a linear model to represent the plant:

$$\bar{x}_{j+1} = \bar{A}\bar{x}_j + \bar{B}\bar{u}_j \qquad \forall j \in \mathcal{J}_0^{N-1} \tag{9}$$

$$\bar{y}_{j,k} = \bar{C}\bar{x}_j + \bar{d}_j \qquad \forall j \in \mathcal{J}_1^{N} \tag{10}$$

where $\bar{A}$, $\bar{B}$ and $\bar{C}$ are state-space matrices. N is the DRTO prediction horizon. $\bar{x}_j \in \mathcal{R}^{n_x}$, $\bar{u}_j \in \mathcal{R}^{n_u}$, $\bar{y}_j \in \mathcal{R}^{n_y}$ are state, input and output vectors, respectively. $\bar{d}_j = y_{j*}^m - \bar{C}\bar{x}_{j*-1,1}$ is a disturbance estimate. Here, $j*$ indicates the current simulation time-step, while j indicates the DRTO time-step. We additonally impose bounds on the states and outputs.

MPC-KKT subproblems: We use the associated first-order (KKT) conditions of the optimization problem in Section 4.2 to account for the lower-level control action in the control-aware scheduling formulation. Because the MPC problem in Section 4.2 is convex, the first-order KKT conditions are necessary and sufficient for optimality. We solve one MPC problem (i.e. a KKT problem) at every time-step j to obtain the input trajectory $u_{j,0}, u_{j,1}, \cdots, u_{j,M-1}$, from which the first element is applied to the process model in (9):

$$\bar{u}_j = u_{j,0}, \quad \forall j \in \mathcal{J}_0^{N-1}$$

The disturbance estimate for the j^{th} MPC-KKT subproblem is computed as $d_j = \bar{y}_j - Cx_{j-1,1}$ for all $j \in \mathcal{J}_1^{N-1}$. That is, the process model prediction $\bar{y}_j$ is used as a surrogate for the measurement y_{j*}^m. For $j = 0$, $d_0 = y_{j*}^m - Cx_{j*-1,1}$.

The MPC-KKT subproblems are additionally linked via

$$x_{j,0} = x_{j-1,1} \qquad \text{and} \qquad u_{j,-1} = u_{j-1,0} \tag{11}$$

for all $j \in \mathcal{J}_1^{N-1}$. Note that the above constraints mimic the closed-loop interaction between the lower-level MPC and the plant.

The set-point y_j^{SP} for every MPC-KKT subproblem constitutes one of the main degrees of freedom for the control-aware scheduling formulation:

$$y_{\min}^{\mathrm{SP}} \leq y_j^{\mathrm{SP}} \leq y_{\max}^{\mathrm{SP}}$$

The subscripts min and max denote lower and upper bounds.

Scheduling constraints: The scheduling constraints are used to define the production sequencing, production amounts, and whether or not the output is meeting the quality specifications. The following constraints specify that only one grade can be produce at any time-step j:

$$\sum_{g \in \mathcal{G}} z_{j,g} \leq 1, \qquad \forall j \in \mathcal{J}_1^{N} \tag{12}$$

where $z_{j,g}$ is a binary variable, and $\mathcal{G} = \{A, B, C\}$ is the set of grades. We use the following to guarantee that $z_{j,g}$ is one only if all outputs are simultaneously within their quality target band for grade g at time-step j

$$\bar{y}_{j,i} \geq \sum_{g \in \mathcal{G}} z_{j,g} \left(y_{g,i}^{target} - \epsilon_{g,i}\right) + (1 - \sum_{g \in \mathcal{G}} z_{j,g})\bar{y}_{\min,i} \tag{13}$$

$$\bar{y}_{j,i} \leq \sum_{g \in \mathcal{G}} z_{j,g} \left(y_{g,i}^{target} + \epsilon_{g,i}\right) + (1 - \sum_{g \in \mathcal{G}} z_{j,g})\bar{y}_{\max,i} \tag{14}$$

$\forall j \in \mathcal{J}_1^N, i \in \mathcal{Y}$. $y_{g,i}^{target} \pm \epsilon_{g,i}$ is the quality target band for grade g and the i^{th} element of the output vector $\bar{y}_j$ (i.e. $\mathcal{Y} = \{1, \ldots, n_y\}$). The subscript min and max indicates lower and upper bounds on the i^{th} output. The inventory level $I_{j,g}$ of grade g at time-step j is given by:

$$I_{j,g} = I_{j-1,g} + z_{j,g}(\Delta t F) - D_{j,g}, \quad g \in \mathcal{G}, j \in \mathcal{J}_1^N \tag{15}$$

$$I_{j,g} \geq 0, \qquad g \in \mathcal{G}, j \in \mathcal{J}_1^N \tag{16}$$

Where $D_{j,g}$ is the product demand, Δt is the MPC sampling time, F is the outlet flow rate of the reactor.

$\Delta t F$ is the amount of product produced at a given time-step j. We impose additional constraints to limit grade transition changes within a each DRTO execution.

Objective function: The objective function is to minimize the input and inventory costs:

$$\Phi = \sum_{j \in \mathcal{J}_0^{N-1}} \left(\sum_{i \in \{1,\ldots,n_u\}} c_i^u \bar{u}_{j,i} + \sum_{g \in \mathcal{G}} c_g^I I_{j,g} \right) \tag{17}$$

where c_i^u and c_g^I are cost coefficients. For improved performance, we augment this objective function with two terms: (1) a soft constraint on the inventory level to encourage inventory build-up (prevent depletion), and (2) a soft constraint on the outputs to prevent them from settling at the boundary of the quality target band during production mode (Dering and Swartz, 2023b).

4.4 Closed-loop simulation

The MPC sampling time is chosen as $\Delta t = 0.1$ h. We also set $P = 15$, $M = 3$, $N = 30$, $Q = \text{diag}(0.01, 1)$, and $R = \text{diag}(1 \times 10^{-6}, 0.1)$. The state-space matrices A, and B for the MPC controller are obtained via linearizaton of the nonlinear process model at $T = 320$ K, $C_A = 1.041$ kmol/m^3, $Q = 2.06 \times 10^4$ kJ/h, and $C_{A0} = 1$ kmol/m^3. The state-space matrices $\bar{A}$ and $\bar{B}$ used at the DRTO level are obtained via linerization of the nonlinear model at $T = 330$ K, $C_A = 3$ kmol/m^3, $Q = 2.15 \times 10^4$ kJ/h, and $C_{A0} = 3.219$ kmol/m^3. We have that $\bar{C} = C = \text{diag}(1, 1)$.

The control-aware scheduler is implemented in AMPL and solved using Gurobi, while the plant and lower-level MPC are implemented using CasADi (Andersson et al., 2019) and solved using IDAS (Gardner et al., 2022) and IPOPT (Wächter and Biegler, 2006), respectively. The actual plant is represented in the overall simulation by the nonlinear model described in (1)-(2). The control-aware scheduling problem is solved at every 0.2 h to compute set-points y_j^{SP} for the lower-level MPC. Only the first two pieces of the DRTO computed set-point trajectory, y_0^{SP} and y_1^{SP}, are assigned to the controller. This is because there are only two MPC executions between consecutive solutions of the control-aware problem. Note also the presence of plant-model mismatch since we utilize a linear process model representation in (9).

The input trajectories computed by the lower-level MPC are presented in Fig. 5, while the simulated plant response is shown in Fig. 6. The dashed lines correspond to the first two pieces of the set-point trajectories computed by the DRTO at every 0.2 h. The quality target bands for each grade are indicated by the shaded area. The inventory of each grade is presented in Fig. 7.

The DRTO-computed set-point trajectories successfully drive the plant to meet the demand of all the grades, and to build-up some inventory, despite the plant-model mismatch.

5. CONCLUSION

We provided an overview of paradigms for integrating scheduling and control, with a special focus on control-aware scheduling formulations. Subsequently, we presented an application case study that demonstrates the use of a control-aware formulation to compute set-point trajectories for the model predictive controller of a nonlinear plant. The calculated set-point trajectories effectively guided the plant to meet the demand for all product grades, even in the presence of structural plant-model mismatch, illustrating the potential of control-aware scheduling formulations.

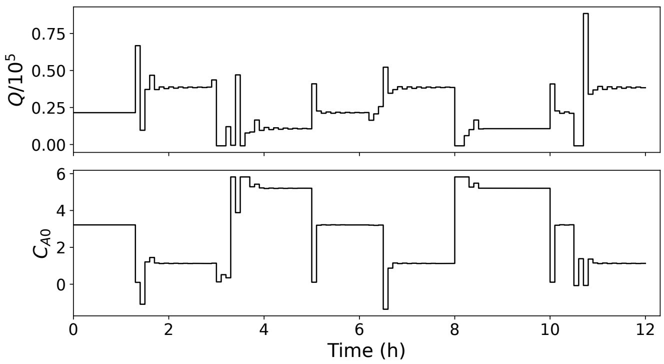

Fig. 5. Heat input Q (kJ/h) and inlet concentration C_{A0} (kmol/m^3).

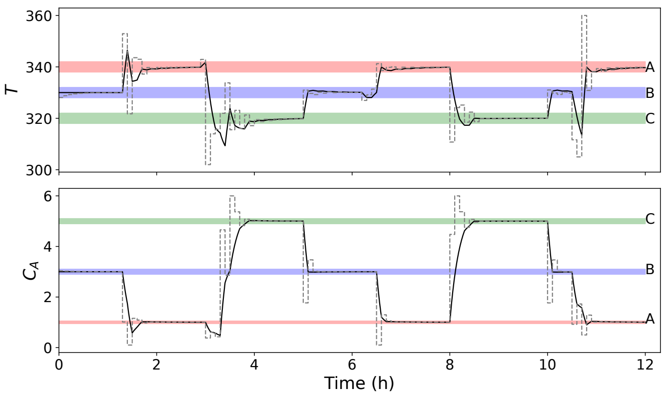

Fig. 6. Reactor temperature T (K) and concentration C_A (kmol/m^3) (solid line), and set-point trajectories (dashed line).

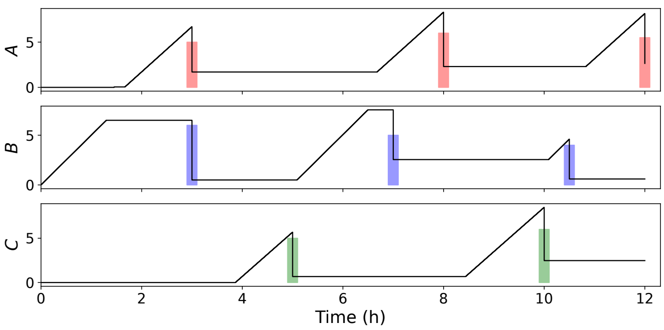

Fig. 7. Inventory trajectory in m^3. The demand is indicated by shaded bars.

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