An Economic Model Predictive Control Approach to Integrated Production Management and Process Operation

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Managing production schedules and tracking time-varying demand of certain products while optimizing process economics are subjects of central importance in industrial applications. We investigate the use of economic model predictive control (EMPC) in tracking a production schedule. Specifically, given that only a small subset of the total process state vector is typically required to track certain scheduled values, we design a novel EMPC scheme, through proper construction of the objective function and constraints, that forces specific process states to meet the production schedule and varies the rest of the process states in a way that optimizes process economic performance. Conditions under which feasibility and closed-loop stability of a nonlinear process under such an EMPC for schedule management can be guaranteed are developed. The proposed EMPC scheme is demonstrated through a chemical process example in which the product concentration is requested to follow a certain production schedule. © 2016 American Institute of Chemical Engineers AIChE J, 63: 1892–1906, 2017

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Introduction

Dynamic product demand changes have made it necessary to increase the operational management efficiency and plant economic performance in the chemical and petrochemical industry. This has led process systems engineers in both academia and industry to develop technologies that aim to economically optimize process operation and allow for real-time energy management. Integrating feedback control strategies with plant economic optimization serves as one approach for achieving optimal process operation. Economic model predictive control (EMPC) is a fairly recent control strategy that integrates dynamic economic plant optimization and a feedback control policy by utilizing an economics-based cost function and the process dynamic model to predict the plant evolution. EMPC has gained attention due to its ability to yield optimal time-varying operation while accounting for operational constraints and ensuring closed-loop stability (e.g., Refs. 1-4).

Production management subject to demand changes plays a crucial role in industry.^{5–8} Shifts in demand and supply of

certain products occur constantly and finding reliable methods to achieve the desired production has become necessary.^{9,10} It has become common in the chemical industry to produce multiple products from the same plant in both batch and continuous processes^{6,8,11} such as the production of multiple grades of polyethylene.¹² Various studies have considered the integration of planning and scheduling in supply chain optimization to achieve economically optimal operational management in response to the desired demand.^{5,8–10} Some methods proposed in this context have been inspired by process control design methodologies, such as modeling the dynamic production in supply chains and using classical process control strategies to manage and control the supply chain.¹³ In addition, several frameworks that use advanced control and optimization strategies have been proposed for scheduling to optimize the decision-making process while accounting for practical constraints and limitations.^{8,9} Furthermore, a rolling horizon approach solved using multiparametric programming with uncertainties in both the disturbances and initial states was investigated for reactive scheduling.¹⁴ Scheduling of industrial electricity use, with a case study for the energy-intensive chlor-alkali process, was also investigated in Ref. 15 by considering contracts between industrial consumers and electricity producers with price penalties in use over the contract in the scheduling problem.

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After solving the planning and scheduling problem, process control strategies are used to drive the plant to follow the desired production schedule. Scheduling and control are two crucial elements that serve the same overall goal of maximizing plant economics while meeting the customer demand. Linking the control problem with the scheduling problem by accounting for the control layer in the scheduling layer to improve economics has been considered.¹⁶ Solving the control and scheduling problems simultaneously while accounting for the nonlinear dynamics of processes to find optimal steadystates and optimal product and state transitions has been considered.^{17,18} Integrating process design with control and scheduling has also been investigated.¹⁹ Considering process dynamics in the scheduling layer through developing scheduling-oriented low-order dynamic models by selecting scheduling relevant variables and using historical data to identify empirical models that capture the dynamic response to production targets has been proposed in Ref. 20. Extensive research efforts have been dedicated recently to developing reliable methods that could track desired production set-points that correspond to different operating conditions.^{6,21,22} The development of a computationally efficient Lyapunov-based scheduling procedure for control of nonlinear systems where each controller is equipped with a Lyapunov function corresponding to a different region of operation has been studied in Ref. 23. Demand management through production scheduling and closed-loop process control while accounting for the cost of transition between different production levels has also been proposed in Ref. 22. This concept can be used for demand response of industrial electricity customers.²⁴ In addition, several studies have considered the use of model predictive control (MPC) in tracking the desired production schedule while accounting for input/output constraints.^{5,6,21} The use of a lowdimensional time scale-bridging model (SBM) in a scheduling-oriented MPC to link control with scheduling and capture the closed-loop dynamics over the longer time scales of the scheduling problem has been considered in Ref. 5. In addition, the use of EMPC for the economic-oriented control and energy management of buildings heating, ventilation, and air conditioning (HVAC) systems has been considered by transforming the scheduling and control problem into a hierarchy of coordinated controllers to deal with the multiple time scale dynamic behavior of buildings, and the complexity that arises from having integer decision variables.²⁵ Integrating scheduling and control for continuous processes under dynamic product demand changes was proposed where a model predictive controller was used to track the schedule set-points.⁶ Another application of combining scheduling with control is for a post-combustion CO₂ capture process.²⁶

Typically, only a subset of the components of the total process state vector is required to follow a production schedule. Therefore, there is a potential in many processes to meet the desired schedule while achieving economically optimal process operation. In this work, we propose an approach that achieves maximizing plant economics while meeting the desired production schedule using EMPC. The EMPC framework tracks production schedules for the desired states while maximizing economics with respect to the rest of the states within manifolds in the process state-space that maintain the requested schedule. Practical considerations that should be introduced at the operating or scheduling level when the EMPC for schedule management is used are discussed. Sufficient conditions for feasibility and closed-loop stability of a nonlinear process under the proposed LEMPC formulation are derived for the case that the times at which the changes in the production level required by the schedule are known *a priori* and the case that they are not. The LEMPC with production schedule management method is applied to a chemical process example and closed-loop simulations demonstrate closed-loop stability of the process while following the desired production schedule and maximizing economics.

Preliminaries

Notation

The symbol x^T is used to denote the transpose of the vector x. The two-norm of a vector is denoted by the operator $|\cdot|$. A continuous function $\alpha : [0, a) \rightarrow [0, \infty)$ is called a class \mathcal{K} function if it is strictly increasing and $\alpha(0)=0$. The symbol Ω_{ρ} is used to denote a level set of a sufficiently smooth scalar function V(x) ($\Omega_{\rho} := \{x \in \mathbb{R}^n : V(x) \leq \rho\}$). The symbol $\Delta > 0$ denotes the sampling period.

Class of systems

The class of nonlinear systems considered in this work is described by nonlinear ordinary differential equations of the following form:

$$\frac{dx}{dt} = f(x, u, w) \tag{1}$$

where $x \in \mathbb{R}^n$ and $u \in \mathbb{R}^m$ are the system state and manipulated input vectors, respectively. The vector $w \in \mathbb{R}^l$ denotes the disturbance vector. Actuator constraints on the control energy available are considered by restricting the control actions to belong to the convex set $U := \{u \in \mathbb{R}^m : u_i^{\min} \le u_i \le u_i^{\max}, i=1,\ldots,m\}$. The disturbance vector is assumed to be bounded (i.e., $w \in W := \{w \in \mathbb{R}^l : |w(t)| \le \theta \forall t\}$). The origin is taken to be an equilibrium of the unforced system of Eq. 1 (i.e., f(0,0,0)=0). At each sampling time $t_k=k\Delta$, $k=0,1,\ldots$, measurements of the state vector $x(t_k)$ are assumed to be available.

The class of nonlinear systems studied is restricted to stabilizable nonlinear systems for which there exists a controller $h(x) \in U$ that can render the origin of the nominal $(w(t) \equiv 0)$ closed-loop system of Eq. 1 asymptotically stable in the sense that there exists a sufficiently smooth Lyapunov function $V: \mathbb{R}^n \to \mathbb{R}_+$ that satisfies the following inequalities^{27,28}:

$$\alpha_1(|x|) \le V(x) \le \alpha_2(|x|), \tag{2a}$$

$$\frac{\partial V(x)}{\partial x}f(x,h(x),0) \le -\alpha_3(|x|),\tag{2b}$$

$$\left|\frac{\partial V(x)}{\partial x}\right| \le \alpha_4(|x|) \tag{2c}$$

for all *x* in an open neighborhood $D \subseteq \mathbb{R}^n$ that includes the origin and $\alpha_j(\cdot)$, j=1, 2, 3, 4, are class \mathcal{K} functions. The stability region of the closed-loop system is taken to be the level set $\Omega_{\rho} \subset D$ where $\dot{V} < 0$. The origin of the system of Eq. 1 is rendered practically stable²⁹ when the controller h(x) is applied in a sample-and-hold fashion for a sufficiently small sampling period. The function *f* is assumed to be locally Lipschitz on $\Omega_{\rho} \times U \times W$.

In this work, it is assumed that the values of the first n_s states of the state vector x (i.e., x_i , $i=1,\ldots,n_s$) are required to be maintained at certain values $x_{i_{desired}}$, $i=1,\ldots,n_s$, which change at specific points in time corresponding to a production schedule. For every set of values $x_{i_{desired}}$, $i=1,\ldots,n_s$, within

the schedule, we assume that a steady-state of the nominal system of Eq. 1 exists at which the states x_i , $i=1,\ldots,n_s$, have the required values. The origin of the system of Eq. 1 can be translated to have its equilibrium at each of these steady-states corresponding to the schedule. We assume that for each steady-state, there exists a stabilizing controller that can make that steady-state asymptotically stable, with a corresponding Lyapunov function. With a slight abuse of notation, we will denote in this article the deviation of the state from the currently desired steady-state by x and will use the notation (e.g., f, V, h, D, Ω_{ρ} , and α_j , j=1, 2, 3, 4) developed in the above discussion for the case that the equilibrium was at the origin of the original system to denote analogous regions or functions for each deviation variable x. With this convention, it is assumed that the Lyapunov function and stabilizing controller for each steady-state satisfy Eq. 2.

Because *f* is Lipschitz continuous, *V* is sufficiently smooth, and *x*, *u*, and *w* are bounded within compact sets, there exist $M > 0, L_x > 0, L_w > 0, L'_x > 0$ and $L'_w > 0$ such that:

$$|f(x, u, w)| \le M \tag{3}$$

$$|f(x_1, u, w) - f(x_2, u, 0)| \le L_x |x_1 - x_2| + L_w |w|$$
(4)

$$\frac{\partial V(x_1)}{\partial x} f(x_1, u, w) - \frac{\partial V(x_2)}{\partial x} f(x_2, u, 0) \bigg| \leq L'_x |x_1 - x_2| + L'_w |w|$$
(5)

for all $x, x_1, x_2 \in \Omega_{\rho}$, $u \in U$, and $|w| \leq \theta$.

Economic model predictive control

EMPC is a MPC strategy for which the objective function is based on economics and does not have its minimum at the economically optimal steady-state of the process (examples of processes for which this may hold true are those which are operated most optimally under a periodic operating policy^{30–33} or those for which other time-varying operating policies that do not necessarily have any pattern or periodicity are economically optimal). To address feasibility and closed-loop stability of a process under such a controller, a variety of constraints have been investigated, but a general formulation of EMPC is as follows³⁴:

$$\min_{u\in S(\Delta)} \int_{t_k}^{t_{k+N}} -L_e(\tilde{x}(\tau), u(\tau)) \ d\tau + V_f(\tilde{x}(t_{k+N}))$$
(6a)

s.t.
$$\dot{\tilde{x}}(t) = f(\tilde{x}(t), u(t), 0)$$
 (6b)

$$\tilde{x}(t_k) = x(t_k) \tag{6c}$$

$$u(t) \in U, \ \forall \ t \in [t_k, t_{k+N}) \tag{6d}$$

$$g(\tilde{x}(t), u(t)) \le 0, \ \forall \ t \in [t_k, t_{k+N}]$$
(6e)

where the stage $\cot L_e(\tilde{x}(\tau), u(\tau))$ (Eq. 6a) represents the process profit, and $V_f(\tilde{x}(t_{k+N}))$ is a terminal penalty evaluated at the predicted state \tilde{x} at the end of the prediction horizon of length N (where the prediction $\tilde{x}(t)$ is the solution of the nominal process model of Eq. 6b at time t given the initial condition of Eq. 6c obtained from a state measurement at time t_k). The constraint of Eq. 6d ensures that the process inputs, which are the decision variables $u(u(\cdot) \in S(\Delta)$ signifies that the decision variables are piecewise constant vectors with period Δ) of the EMPC meet the input constraints. The function g(x, u) represents any additional constraints that may be included within the EMPC. Three constraints that are often used within EMPC for stability purposes and can be represented by g are a terminal equality constraint,³⁵ a terminal region constraint,¹ and Lyapunov-based constraints³ (for the terminal equality constraint and Lyapunov-based constraints, V_f is not usually included³⁴). Other types of constraints or considerations for EMPC are addressed in Refs. 2 and 34.

Lyapunov-based EMPC

Although this work will address scheduling management in the context of EMPC in general, the formulation of EMPC with Lyapunov-based stability constraints (termed Lyapunovbased EMPC (LEMPC)³) will receive special focus because it is straightforward for this method to prove feasibility and closed-loop stability of a process under this EMPC formulation in the presence of disturbances with an *a priori* characterization of the set of initial conditions for which recursive feasibility is guaranteed. The formulation of LEMPC, incorporating Lyapunov-based stability constraints based on the explicit controller h(x), is as follows:

$$\min_{u\in S(\Delta)} \int_{t_k}^{t_{k+N}} -L_e(\tilde{x}(\tau), u(\tau)) \ d\tau \tag{7a}$$

s.t.
$$\dot{\tilde{x}}(t) = f(\tilde{x}(t), u(t), 0)$$
 (7b)

$$\tilde{x}(t_k) = x(t_k) \tag{7c}$$

$$u(t) \in U, \ \forall \ t \in [t_k, t_{k+N})$$
(7d)

$$V(x(t)) \leq \rho_e, \quad \forall \ t \in [t_k, t_{k+N})$$

if $x(t_k) \in \Omega_{\rho_e}$ (7e)

$$\frac{\partial V(x(t_k))}{\partial x} f(x(t_k), u(t_k), 0) \\
\leq \frac{\partial V(x(t_k))}{\partial x} f(x(t_k), h(x(t_k)), 0) \\
\quad \text{if } x(t_k) \notin \Omega_{\rho_e}$$
(7f)

where the notation follows that in Eq. 6. When a state measurement is received, either the Mode 1 (Eq. 7e) or the Mode 2 (Eq. 7f) constraint is activated based on the state location in the state-space. Mode 1 promotes time-varying operation to maximize profit while maintaining the state within the region $\Omega_{\rho_e} \subset \Omega_{\rho}$. Mode 2 is activated when the closed-loop state escapes the Ω_{ρ_e} region to force the state back into Ω_{ρ_e} by computing control actions that decrease the Lyapunov function value. Ω_{ρ_e} is chosen to make Ω_{ρ} forward invariant in the presence of disturbances. For additional discussion of LEMPC and a more rigorous closed-loop stability analysis, the reader can refer to Ref. 3. The control actions calculated from the LEMPC design are applied in sample-and-hold in a receding horizon fashion.

Remark 1. The characterization of V and Ω_{ρ_e} is crucial to the development of the LEMPC of Eq. 7. There is not a general method for determining which Lyapunov function candidate (positive definite function with V(0)=0) will be a Lyapunov function for a given nonlinear system (i.e., cause Eq. 2 to be satisfied for the nonlinear system), but quadratic Lyapunov functions have generally been successful.³⁶ Also, some works have developed methods for obtaining Lyapunov functions for certain systems.³⁷ The determination of Ω_{ρ_e} can be made through closed-loop simulations of the nonlinear process under the Lyapunov-based controller with simulated disturbances (based on knowing the bound θ on the magnitude of the disturbance). Methods for obtaining a

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Lyapunov-based control law for use in evaluating Ω_{ρ_e} through this methodology are addressed in references such as Refs. 29, 36 and 38–40.

Schedule Management Using EMPC

In this section, we discuss the formulation of the proposed EMPC for schedule management, along with practical and theoretical considerations. We will refer to the states that are required to follow a certain schedule as the scheduled states, and to those that do not have this requirement as the free states.

Formulation of EMPC for schedule management

In this section, we present several ideas for formulating an EMPC for schedule management, all of which are designed to meet the constraint of the scheduling problem (i.e., the first n_s states x_i , $i=1,...,n_s$, of the state vector are required to be maintained at desired values $x_{i_{desired}}$, $i=1,...,n_s$), while simultaneously varying the remaining $n-n_s$ free states in a manner that optimizes the process economics and ensures satisfaction of all process constraints. Using the EMPC framework, meeting the schedule is thus considered to be a constraint on some states, rather than the goal of process operation. As noted in the section "Class of systems," we assume that the origin of the system of Eq. 1 is translated to be at a steady-state where the schedule is met so that $x_{i_{desired}}=0$, $i=1,...,n_s$.

To illustrate the manner in which the free states may vary to maximize process economics while the scheduled states satisfy the requested schedule, Figure 1 presents an example with three states (x_1, x_2, x_3) , in which the state x_1 must follow a certain schedule. The original steady-state is at the origin, and $x_{1_{desired}} = 0$. The process is initially operated in a manner that keeps x_1 small while allowing x_2 and x_3 to vary to maximize the process economics. At t_1 , the state is at the dot on the x_3 axis, and the scheduled value for x_1 changes from $x_1=0$ to a new value of x_1 that corresponds to the x_1 value of the plane to the right of the origin in Figure 1. As illustrated in this figure, the state is driven to this plane to meet the required schedule, and then moves around within the plane to optimize the process economics while continuing to meet the schedule.

Perhaps the most intuitive EMPC formulation for schedule management is one that uses a hard constraint for the scheduled states to enforce that they must meet the schedule at all times (except for a time during the transient between two steady-states), with either a terminal equality constraint or terminal region constraint (as g(x, u) in Eq. 6) around the steadystate corresponding to the scheduled values for stability purposes. This allows the free states to maximize process economics as long as they reach the steady-state values at the end of the prediction horizon. Although this method of enforcing the schedule as a hard constraint is intuitively appealing because it ensures that the schedule can be met for a system without disturbances when the problem is feasible, it may result in feasibility issues at a plant where plant-model mismatch, measurement noise, and process disturbances are unavoidable. To avoid this, the schedule constraints discussed above could be implemented as soft constraints. In such a case, however, the set of initial conditions from which feasibility and closed-loop stability of a process under the EMPC could be proven would not be as straightforward to obtain as when the soft constraints are utilized in the context of LEMPC (Eq. 7), so the details of an LEMPC formulation for schedule management will be the subject of the rest of this section.



Figure 1. Illustration of a possible state trajectory for the closed-loop process under the EMPC for schedule management.

The process is initiated from the dot on the x_3 axis and subsequently travels along the dotted line to the plane on the right of the figure in which x_1 is fixed, driving x_1 to the value required by the schedule. The state subsequently moves within the plane of fixed x_1 (solid line in the figure) to maximize the process economics with the remaining states while continuing to meet the schedule.

The formulation of an LEMPC that achieves the scheduling objective using a soft constraint on the schedule (i.e., the LEMPC seeks to drive the n_s states x_i , $i=1,\ldots,n_s$, quickly to the values required by the production schedule and to maintain the states close to $x_{i_{desired}}$, $i=1,\ldots,n_s$, thereafter) is as follows:

$$\min_{u\in S(\Delta)} \int_{t_k}^{t_{k+N}} -L_e(\tilde{x}(\tau), u(\tau)) + \sum_{i=1}^{n_s} \alpha_{Wi}(\tilde{x}_i(\tau))^2 d\tau \qquad (8a)$$

s.t.
$$\dot{\tilde{x}}(t) = f(\tilde{x}(t), u(t), 0)$$
 (8b)

$$\tilde{x}(t_k) = x(t_k) \tag{8c}$$

$$u(t) \in U, \ \forall \ t \in [t_k, t_{k+N})$$
(8d)

$$V(\tilde{x}(t)) \le \rho_e, \ \forall \ t \in [t_k, t_{k+N})$$
(8e)

$$\text{if } x(t_k) \in \Omega_{\rho_e}$$

$$\frac{\partial V(x(t_k))}{\partial x} f(x(t_k), u(t_k), 0)$$

$$\leq \frac{\partial V(x(t_k))}{\partial x} f(x(t_k), h(x(t_k)), 0)$$
if $x(t_k) \notin \Omega_{\rho_e}$ or $|x_i(t_k)| \geq \gamma_i$, $i=1,\ldots,n_s$, (8f)
or $t_k > t'$

where the notation follows that in Eq. 7. The LEMPC cost function consists of two components: the first component $L_e(\tilde{x}(\tau), u(\tau))$ represents the process profit, and the second component penalizes deviations of the states x_i , $i=1,\ldots,n_s$, from the desired values $x_{i_{desired}}=0$, $i=1,\ldots,n_s$. The weighting coefficients α_{Wi} , $i=1,\ldots,n_s$, can be chosen to obtain a desired trade-off between optimizing the process economics and the rate of approach of the scheduled states to the scheduled values. The time t' in the constraint of Eq. 8f will be discussed in later sections.

The states of a process operated under the LEMPC of Eq. 8 that are required to meet a schedule must be maintained sufficiently close to the desired values to meet the schedule, and

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also must never leave the stability region Ω_{ρ} to ensure closedloop stability. The Mode 1 and Mode 2 constraints in Eqs. 8e and 8f ensure that both of these requirements are met. As in Eq. 7, the Mode 2 constraint is activated when the measurement of the closed-loop state at t_k is outside of Ω_{ρ_e} , which ensures that the state never leaves Ω_{ρ} . In addition, because the first n_s states meet their production schedule at the origin, and repeated application of the Mode 2 constraint drives the closed-loop state to a small neighborhood $\Omega_{\rho_{\min}}$ of the origin,³ the Mode 2 constraint is also activated whenever the measured value of any state that is required to meet a schedule deviates from this schedule by more than an allowable amount γ_i , $i=1,\ldots,n_s$. This ensures that any deviation from the schedule causes the state to be driven back toward the origin, where all required states are within γ_i , $i=1,\ldots,n_s$, and the schedule is thus sufficiently followed (this is guaranteed only if each γ_i is greater than or equal to the maximum magnitude of the corresponding state x_i in $\Omega_{\rho_{\min}}$ because then the contractive constraint can drive the closed-loop state into a region $\Omega_{
ho_{\min}}$ where the scheduled states are no more than γ_i from their scheduled values). When $t_k \ge t'$, the Mode 2 constraint is applied regardless of the location of the state measurement $x(t_k)$ within Ω_{ρ} . This corresponds to successive application of the Mode 2 constraint, which will drive the closed-loop state into $\Omega_{\rho_{\min}}$ and maintain it there thereafter. Whenever the Mode 2 constraint is active but $x(t_k) \in \Omega_{\rho_a}$, the Mode 1 constraint is simultaneously active (which particularly impacts the trajectories for the last N-1 sampling periods of the prediction horizon which are unaffected by the contractive constraint that is applied in only the first sampling period of the prediction horizon).

When the state measurements at t_k of the first n_s states are within γ_i , $i=1, \ldots, n_s$, of their scheduled values, the full process state is within Ω_{ρ_e} , and $t_k < t'$, the Mode 1 constraint is active, and the Mode 2 constraint is not applied. This allows control actions to be computed that vary the unscheduled states throughout Ω_{ρ_e} to achieve economic optimality while meeting the schedule. If the weights α_{Wi} , $i=1,\ldots,n_s$, are appropriately chosen, the LEMPC will choose control actions that prevent the values of x_i , $i=1,\ldots,n_s$, from becoming large, which means that the economic optimization will primarily adjust the $n-n_s$ states that do not need to follow a schedule to attain economic optimality while continuing to keep the x_i , $i=1,\ldots,n_s$, close to their scheduled values.

Remark 2. We note that production schedules often set target values for process outputs/quality variables. In most chemical process systems, the process outputs/quality variables are a subset of the components of the system state vector. In this work, we assume that full state feedback is available because the economics-based objective function of EMPC typically depends on some (if not all) of the process states. In this case, the measurements of the states that are required to meet the schedule are readily available as process outputs (an alternative method for implementing EMPC when full state feedback is not available, i.e., only some state measurements are available, is to use a state estimation technique such as robust moving horizon estimation to obtain estimates of the unmeasured states which could include scheduled states; however, this requires an output feedback EMPC design,⁴¹ which is not rigorously developed in this article). Throughout the article, we have assumed that the outputs/quality variables that are required to meet the schedule are process states, and as a result, no output function was required in Eq. 1. However, the methodology presented in this article can be extended to the case that the production schedule requires that some linear or nonlinear combination of the state variables track specific values. In that case, a steady-state corresponding to values of the states at which the schedule is met for the combination outputs can still be defined, and the controller formulation presented in Eq. 8 can be redesigned to enforce that the combination outputs meet the schedule (by utilizing the weights in the objective function on the deviations of the combination outputs from their required values instead of imposing these weights on the individual state variables).

Remark 3. The claim that an EMPC for schedule management that does not have Lyapunov-based stability constraints like the LEMPC for schedule management in general would be more difficult to analyze for closed-loop stability and feasibility properties than the LEMPC of Eq. 8 deserves some further discussion. The closed-loop stability and feasibility properties of EMPC's of the form of Eq. 6 with constraints such as terminal equality³⁵ and region constraints¹ have been characterized in the literature for nominal $(w(t) \equiv 0)$ operation. However, the region from which initial feasibility (which is a prerequisite for the closed-loop stability results) is guaranteed is difficult to characterize a priori. For example, in the terminal equality constraint formulation, the set of conditions which guarantee initial feasibility is the set from which the EMPC is able to find a solution that causes all state constraints to be met throughout the prediction horizon. Since EMPC is typically formulated with a nonlinear process model, the regions accessed by the closedloop states under any sample-and-hold input policy can generally only be determined through closed-loop simulations. Therefore, the control actions that will cause the state predictions from the process model to satisfy the state constraints throughout the prediction horizon cannot in general be determined a priori (i.e., closed-loop simulations under the EMPC are required to determine them). Furthermore, because the feasibility results can only be guaranteed when $w(t) \equiv 0$, recursive feasibility is not guaranteed in the presence of plant-model mismatch/disturbances, so determining the set of points from which recursive feasibility holds in the presence of disturbances also cannot be easily characterized for these formulations. LEMPC,³ however, is designed so that an explicit Lyapunov-based controller implemented in sample-and-hold is always a feasible solution to the optimization problem even in the presence of disturbances/plantmodel mismatch as long as the magnitude of the disturbances/plant-model mismatch and the length of the sampling period are sufficiently small. This is guaranteed through the design of the stability region utilizing the Lyapunov-based controller implemented continuously and the robustness properties of the Lyapunov-based controller when implemented in sample-and-hold that allow the Lyapunov-based controller implemented in sample-and-hold to maintain the closed-loop state within the stability region for sufficiently small sampling periods and sufficiently small disturbances.²⁵ Furthermore, because the Lyapunov-based controller is a feasible solution from any initial condition within the stability region and LEMPC maintains the closed-loop state within the stability region at all times, the LEMPC is guaranteed to be recursively feasible even in the presence of disturbances. In addition, the set of initial conditions from which initial and recursive feasibility are guaranteed are those initial conditions within the stability region (i.e., they can be explicitly characterized *a priori*). Because all state-space points within the stability region thus guarantee closed-loop stability and also feasibility even in the presence of disturbances, LEMPC has the unique properties desired for the EMPC for schedule management problem. Specifically, it allows the region from which closed-loop stability and feasibility can be guaranteed for a given steady-state corresponding to a desired production level in the schedule to be characterized (it can be characterized as all state-space points within the stability region of that steady-state is desired and when the steady-state is newly requested due to a change in the production level required by the schedule.

Remark 4. Although it is intuitively desirable to enforce a constraint in Eq. 8 that once the predicted state reaches the scheduled value, it must be maintained at that scheduled value, this would create a hard constraint that cannot be guaranteed to be feasible because the set where $|x_i| \le \gamma_i$, $i=1, \ldots, n_s$, is not an invariant set (although a level set where such conditions are met is an invariant set but may be small).

Schedule changes under EMPC for schedule management

Regardless of the formulation chosen for the EMPC for schedule management (Eq. 6 incorporating a terminal equality constraint or terminal region constraint with a hard constraint for the scheduled states, or a soft constraint formulation on the schedule in the form of Eq. 6 or Eq. 8), a key feature of the EMPC is that it must be capable of handling changes in $x_{i,desired}$, $i=1,\ldots,n_s$, according to the schedule to meet changes in demand or product or resource pricing. For all of the EMPC formulations, this requires a change in the objective function and/or constraints of the problem. Specifically, the terminal region or equality constraints and schedule constraint will be updated if a hard constraint formulation is used, penalties on deviations from the schedule will be updated in the objective function if a soft constraint is used, or the Lyapunov-based constraints will be reformulated with respect to the Lyapunov-based controller for the new steady-state if the LEMPC of Eq. 8 is used. The time at which this change is required may or may not be known by the controller *a priori*. Thus, some consideration must be made for the EMPC for schedule management to determine the manner in which the switching of the control problem should occur to avoid feasibility issues, both when the controller has prior knowledge of the switching time and when it does not.

As mentioned previously, an EMPC formulation for schedule management of the form of Eq. 6 but with either soft or hard constraints on the schedule and terminal equality or region constraints is difficult to evaluate for feasibility considerations when operated for a process without a change in the production level required by the schedule. This is a limitation once again when the production level required by the schedule changes because the set of points for which recursive feasibility is guaranteed in the presence of process disturbances is difficult to characterize. In addition, the set of initial conditions from which the EMPC to be implemented after the production level required by the schedule changes will be feasible is also difficult to characterize, so the question of when it is possible to change to the next production level required by the schedule



Figure 2. Illustration of intersection of level sets corresponding to each steady-state where the process schedule is met.

while maintaining feasibility of the control problem is difficult to answer even for nominal operation. However, for the LEMPC of Eq. 8, the conditions under which closed-loop feasibility can be maintained when the time at which it is desired to change $x_{i,desired}$ is known in advance by the controller and when it is not can be explicitly derived.

When the LEMPC begins to drive the closed-loop state to a steady-state at which new values of the scheduled states are met, the LEMPC of Eq. 8 is updated so that it is written with respect to the Lyapunov-based controller and process model with the origin at the steady-state corresponding to the new desired values of the scheduled states. For a feasible solution to the LEMPC for schedule management to be guaranteed when this updated LEMPC begins to be used, the closed-loop state must be contained within the stability region of the new steady-state when the LEMPC being utilized is updated. To see this, suppose that the LEMPC of Eq. 8 is designed with respect to a certain steady-state and is denoted as $LEMPC_1$, and has stability region Ω_{ρ_1} . At time t_1 , the LEMPC will be updated so that it maintains the closed-loop state within the stability region around a new steady-state for which the corresponding LEMPC is denoted $LEMPC_2$ and is the LEMPC of Eq. 8 but with the parameters updated for the new steady-state (e.g., the stability region is Ω_{ρ_2}). To ensure that $x(t_1) \in \Omega_{\rho_1}$ and $\Omega_{
ho_2}$ to guarantee that there is a feasible solution to LEMPC₂ at t_1 , the stability regions for LEMPC₁ and LEMPC₂ must intersect at $x(t_1)$ to ensure that closed-loop stability is maintained at this state under both $LEMPC_1$ and $LEMPC_2$.

Figure 2 illustrates the overlapping of the level sets just described for the case that three changes in the production level required by the schedule occur. The steady-states are denoted as X_{s1} , X_{s2} , and X_{s3} , with corresponding stability regions Ω_{ρ_1} , Ω_{ρ_2} , and Ω_{ρ_3} . In the figure, it is assumed that the process is driven to each steady-state and then operated very close to that steady-state for some period of time. This means

that at t_1 , the state at t_1 (which is the steady-state corresponding to the prior desired value of the scheduled states) must be within the stability region of the new steady-state (e.g., $X_{s2} \in \Omega_{\rho_1}$ and Ω_{ρ_2} , and $X_{s3} \in \Omega_{\rho_2}$ and Ω_{ρ_3}) to ensure feasibility and closed-loop stability of the process.

Ideally, the LEMPC would be updated to start driving the process state toward the next steady-state in the schedule at the switching time t_s at which it is desired to start producing $x_{i,desired}$, $i=1,\ldots,n_s$, at the values corresponding to this new steady-state (i.e., ideally, $t_1 = t_s$, where t_s is defined as the time at which it is desired that the LEMPC begins to drive the closed-loop state toward a new steady-state at which a new production level in the schedule is met, and t_1 is the time at which the LEMPC is actually reformulated to drive the closed-loop state to the new steady-state). However, because feasibility of the optimization problem at t_1 is ensured only if $x(t_1) \in \Omega_{\rho_1}$ and Ω_{ρ_2} , it is only possible for $t_1 = t_s$ when the LEMPC knows t_s far enough in advance to be able to drive the state into $\Omega_{\rho_1} \cap \Omega_{\rho_2}$ before t_s . This is because LEMPC allows time-varying operation, so without the LEMPC taking a specific action to drive the closed-loop state into $\Omega_{\rho_1} \cap \Omega_{\rho_2}$ by t_s , there is no guarantee it is within this region at t_s . If, for example, the LEMPC has no knowledge of t_s until t_s , the LEMPC may need to drive the state into $\Omega_{\rho_1} \cap \Omega_{\rho_2}$ after t_s , so that t_1 may be greater than t_s and thus there may be periods of time during which it is desired to start operating the process at the next $x_{i,desired}$, $i=1,\ldots,n_s$, but this cannot yet occur while maintaining controller feasibility. More will be said regarding a method for choosing Ω_{ρ_2} to ensure that a region $\Omega_{\rho_1} \cap \Omega_{\rho_2}$ exists into which the LEMPC can be guaranteed to drive the process state in finite time in the section "Feasibility and stability analysis." The requirement of overlapping level sets can be relaxed in practice, but feasibility and closed-loop stability then can no longer be guaranteed.

Scheduling and operations considerations with EMPC for schedule management

Several practical considerations for EMPC for schedule management that must be accounted for either at the scheduling level or at the operations level when developing the set of steady-states, Lyapunov-based control laws, and level sets to send to the controller are as follows:

• The EMPC for schedule management requires that a region exists in which the EMPCs designed for both the current and next steady-states are both feasible, and that the state can be driven by the EMPC for schedule management into this region.

Notwithstanding that it may be possible for a variety of EMPC formulations to meet this criterion in practice even if it is not easily provable theoretically, for provable feasibility of the EMPC scheduling problem, the LEMPC formulation should be used and the feasibility issue should be addressed at the scheduling or operations level, depending on the difference between the time scale on which the production level required by the schedule changes and the time scale of the process dynamics, and depending on the impact of the transient on the profit of the process.

When the process dynamics are determined to be on a time scale comparable to the time scale on which the production level required by the schedule changes, or the manner in which transitions between regions of state-space occur is determined to significantly affect the process economics in a manner that would alter the schedule chosen if it were taken into account, it may be desirable to include considerations related to the process dynamics and level set intersections in the scheduling problem. The scheduling problem is often formulated as a mixed-integer linear program, but could be modified to include some representation of level set intersection (e.g., if the level sets are determined a priori, then constraints could be devised that permit the next steady-state in the schedule to only be one for which the level sets intersect; this ensures that, for example, a schedule developed for the steady-states in Figure 2 does not request the production of X_{s1} followed immediately by the production of X_{s3} because Ω_{ρ_3} does not contain X_{s1}). It may be that one or more of the level sets that are found for the steady-states corresponding to demanded products do not intersect any of the other level sets corresponding to demanded products. In this case, it may be necessary to develop additional state-space points which do not correspond to any marketable product but which have level sets that allow for any gaps in state-space where the level sets of the demanded products do not intersect to be bridged. If this is required, such intermediate points can also be considered for inclusion in the scheduling problem, possibly with constraints that try to limit the time spent approaching these intermediate points or the number of intermediate points approached in the schedule. For example, if a schedule requires production only of X_{s1} and X_{s3} in Figure 2 without the production of X_{s2} , then it is not necessary to use the LEMPC for schedule management with the desired steady-state at X_{s2} all the way until the state reaches X_{s2} . Rather, the LEMPC with the desired steady-state at X_{s2} can be applied for an amount of time that ensures that the closed-loop state enters Ω_{ρ_3} , and then the LEMPC with the desired steady-state at X_{s3} can be applied. Because it may be necessary, for example, to produce a product that is not in immediate demand to transition between the production of two more heavily demanded products, accurate forecasting of data used to set the schedule (e.g., demand and pricing) sufficiently long in advance are essential for determining an appropriate schedule for this LEMPC strategy, so that frequent changes to the schedule (i.e., making new schedules for the process/rescheduling production) can be avoided, particularly if the changes require intermediate products to be produced. The scheduling problem may also include a representation of the process dynamics if it is on a time scale comparable to that on which the production level required by the schedule changes, to choose the best schedule accounting for the time spent with off-specification production due to the process dynamics.

If the process dynamics are much faster than the time scale on which scheduling changes occur, it may be decided to relegate the issue of moving between level sets to an operational issue after the schedule is determined. Thus, a standard scheduling problem can be solved without knowledge of the process dynamics or intersecting level sets, but then before sending the steady-states corresponding to the various desired production levels to the controller, the set of steady-states can be evaluated to determine whether their level sets intersect or whether it is necessary to add additional intermediate steady-states to the operating procedure as noted in the prior paragraph to drive the state through state-space without losing controller feasibility. If the time of switching from each production level to the next is known, this can also be considered in the development of the set of steady-states used in the operating procedure so that the production stays as close to the target values that were determined by the scheduling problem for the lengths of time determined by this problem as possible.

• *EMPC* for schedule management in general cannot guarantee that scheduled states are at their values for all time.

Although this may at first seem to be a limitation of the method, when the production level required by the schedule is changed under any controller, there will be some length of time in which the process state is transitioning to its new value at a speed limited by the process dynamics. In addition, if it is required to drive the state into the intersection of the level sets for the prior and new steady-states (e.g., t_s is not known a priori), there will be some time required after the new production level required by the schedule is requested not only to move to the new production level, but also to move toward the region of intersection, and this time cannot be known a priori without closed-loop simulations. In general, the soft constraint formulation offers the flexibility to highly penalize the deviation of the states from the scheduled values so that the EMPC will calculate control actions that attempt to move the process state as quickly as possible to the new steady-state, given the process dynamics. In the presence of disturbances, there is no controller that can keep the values of some or all states at precise values for all times, but high penalties would again cause an EMPC for schedule management to drive the predicted state (and ideally the actual closed-loop state) toward a region where the schedule is met quickly. For the LEMPC for schedule management, because the feasible region is characterizable a priori, closed-loop off-line simulations can be used to estimate a worst-case rate of approach to the next scheduled steady-state. If there are concerns regarding the time that the process is not operating with the states at the schedule due to disturbances, simulations can be performed to evaluate the effect of the choice of γ_i on product quality in the presence of the expected bounded disturbances.

• EMPC for schedule management requires a steady-state to be chosen for the process among many where the values of only the first n_s states are specified.

The steady-state to operate around may be chosen as the economically optimal steady-state at which the schedule is met, subject to practical constraints (e.g., limitations on the temperature for safety reasons).

• The LEMPC for schedule management has tuning parameters α_{Wi} and γ_i , $i=1, \ldots, n_s$, which must be determined before the LEMPC can be utilized and which will affect both schedule tracking and process economic optimization.

The choice of α_{Wi} affects how fast the closed-loop system state approaches a desired production level. Larger values of α_{Wi} drive the scheduled states more quickly to their scheduled values (they more strongly emphasize meeting the schedule compared to optimizing the process economics) than do smaller values of α_{Wi} , which may cause the scheduled states to approach their value more slowly because the economic measure in the objective function would have more of an effect on the LEMPC solution (smaller values of α_{Wi} more strongly emphasize process economics compared to meeting the schedule). Depending on the product that corresponds to a given operating point in the production schedule, the weights may be different for one scheduled production level than for another based on these trade-offs. In addition to accounting for process economics and the schedule, the selected value of α_{Wi} should prevent unfavorable operating strategies. For example, it may not be favored in some cases to have a very large α_{Wi} if that causes large changes in the inputs calculated by the LEMPC between two sampling periods, which may be undesirable for many applications due to the potential of such an operating strategy to cause, for example, actuator wear.

The rate at which the scheduled states approach the schedule for a given value of α_{Wi} , and the types of undesirable operating strategies that may be set up for various values of α_{Wi} , will depend on factors such as the process dynamics and the magnitude of the economics-based term in the objective function. For this reason, closed-loop simulations from a variety of initial conditions and with different values of α_{Wi} can be helpful in assessing the appropriate values of α_{Wi} to achieve the desired trade-offs. The contractive constraint of Eq. 8f ensures that the LEMPC for schedule management will drive the closed-loop state into a region where the magnitude of each scheduled state is within γ_i of its scheduled value regardless of the magnitude of α_{Wi} . However, the role of α_{Wi} is to provide a means for improving the rate of approach of the scheduled states to their scheduled values when desired. Larger values of α_{Wi} (higher penalty on schedule deviations than on economic sub-optimality) may also help prevent the LEMPC from calculating control actions that drive the x_i , $i=1,\ldots,n_s$, off of the scheduled values to improve the process economics.

With regard to the choice of γ_i , because it is impossible for any controller (not only the LEMPC for schedule management) to maintain the process states exactly at a desired value for all times due to both process disturbances and the time required to move between different production levels when requested by the schedule, we assume that deviations of the scheduled state variables from their targets are acceptable as long as the overall product to be sold from the process (which may be a time-averaged quantity if there are mixing or blending steps later in the process) has an acceptable quality (i.e., it is marketable because its quality is within an acceptable range of values around a target production level). To keep the process states sufficiently close to their scheduled values (by activating Mode 2 when $|x_i| \ge \gamma_i$, $i=1,\ldots,n_s$ in an effort to maintain the overall product quality within an acceptable range, the tuning parameter γ_i in the LEMPC for schedule management can be adjusted. However, the relationship between γ_i and the overall product quality is not straightforward (unless the profit potential of EMPC is severely reduced as will be described below). The reason for this is that the contractive constraint is only guaranteed to drive the closed-loop state from one Lyapunov level set into a Lyapunov level set closer to the steady-state; it makes no guarantees regarding whether a specific state x_i , $i=1,\ldots,n_s$, will move closer to or further from its steady-state value within a sampling time, but only guarantees that in finite time the Lyapunov level set shrinks and thus the value of x_i will eventually move closer to its steady-state value. This means that when the magnitude of the deviation of a scheduled state variable from its steady-state value is more than γ_i , which activates Mode 2 operation of the LEMPC for schedule management, it is not known a priori whether the value of x_i will immediately evolve toward its steady-state value or at first move further from this value. The only means for ensuring that each x_i , $i=1,\ldots,n_s$, remains within a specific range of values (after it reaches the schedule; the magnitude of γ_i is not used to drive the closed-loop state toward the steady-state more quickly at a change in the production level required by the schedule as α_{Wi} can) is to define the range of values for each scheduled state, and then to set each γ_i to the maximum magnitude that each x_i can take while maintaining the closed-loop state within a Lyapunov level set

where the required range of values for every x_i is satisfied even in the presence of disturbances (this corresponds to the case that γ_i is defined based on product quality constraints). This Lyapunov level set may be small, reducing the region in state-space within which the LEMPC for schedule management can maximize the process economics utilizing the unscheduled states. This is also an unnecessarily restrictive method of achieving the desired product quality; for example, short excursions of the instantaneous product concentration above its minimum or maximum time-averaged value may still result in an acceptable time-averaged concentration as long as the instantaneous product concentration is below the limits on its range at other times. Less restrictive process operation due to such considerations may improve the process profit by allowing greater flexibility in the operating strategy, while still resulting in an overall acceptable product.

Based on this, it is in general not desirable to set γ_i based on the product quality constraints, but instead to determine which values of γ_i cause the product quality constraints to be met. This determination can be made using process data and closed-loop simulation results for different values of γ_i . This information can indicate which combination of γ_i , $i=1,\ldots,n_s$, values provides optimum process economics by allowing the unscheduled states to move most freely around the steadystate, while still resulting in an overall acceptable product quality (i.e., this analysis evaluates the effect of γ_i on product quality to determine a suitable value of this parameter). Process disturbances should also be accounted for in this analysis. If γ_i is very small relative to regular deviations of the scheduled states from their scheduled values due to process disturbances, the Mode 2 constraint may be triggered almost constantly because of process disturbances, which would enforce steady-state operation and not allow for the possible economic benefits of LEMPC for schedule management. It may be desirable to choose γ_i in a manner that prevents Mode 2 from activating regularly due to common disturbances if this does not significantly affect the product quality.

An implication of the above analysis is that to use the LEMPC for schedule management, the desired product quality must, at minimum, be met during consistent operation within $\Omega_{\rho_{\rm min}}$. If it is not, the LEMPC sampling period can be decreased to decrease $\Omega_{\rho_{\rm min}}$ (although the upper bound on the disturbances also affects the minimum size of $\Omega_{\rho_{\rm min}}$, and that cannot be adjusted).²⁹

The above heuristics can be utilized to help choose values of α_{Wi} and of γ_i either during the scheduling phase or the operations phase. If strict quality requirements are being set by the schedule (or would be desirable but it is unclear whether they can be achieved), it may be necessary to evaluate at the scheduling level whether the proposed quality requirements are reasonable given the process dynamics and expected process disturbances by utilizing closed-loop simulations with different values of α_{Wi} and of γ_i to determine whether the schedule can be met before it is sent to the operations level. If the quality requirements are believed to be reasonably achievable, then α_{Wi} and γ_i can be evaluated for each production level in the schedule at the operations level after the schedule has been set.

• The time length for which a given production rate should be maintained is limited by the closed-loop process dynamics under the LEMPC for schedule management.

The LEMPC for schedule management drives the closedloop state from one scheduled state to the next at a rate that depends on the process dynamics, state and input constraints, and the objective function (i.e., this rate is a closed-loop property). The changes in the desired values of the scheduled states corresponding to desired products cannot be more rapid than the rate at which the closed-loop state is driven between the production levels. If rapid changes in the desired values of the scheduled states are desirable, it may be necessary to evaluate whether the closed-loop process dynamics can be made fast enough to move between production levels in the schedule at the desired rate. This can be accomplished at the scheduling level by tuning α_{Wi} , incorporating closed-loop dynamics within the scheduling problem to evaluate whether the expected rate of approach to the next desired production level in the schedule under the LEMPC is sufficient and cause the schedule to be set based on the closed-loop process dynamics, or by assuming the worst-case rate of approach to the next desired production level in the schedule and using this as a hard constraint on the time required for each production level in the schedule to be maintained.

Feasibility and stability analysis

In this section, we prove feasibility and closed-loop stability of a process under the proposed LEMPC for schedule management. We first present two propositions required for the feasibility and stability proofs, and then present a theorem on the feasibility and stability results.

Proposition 1. (cf. Refs. 3 and 42). Consider the systems

$$\dot{x}_a(t) = f(x_a(t), u(t), w(t)) \tag{9a}$$

$$\dot{x}_b(t) = f(x_b(t), u(t), 0)$$
 (9b)

with initial states $x_a(t_0) = x_b(t_0) \in \Omega_{\rho}$. There exists a \mathcal{K} function $f_W(\cdot)$ such that

$$|x_a(t) - x_b(t)| \le f_W(t - t_0) \tag{10}$$

for all $x_a(t), x_b(t) \in \Omega_\rho$ and all $w(t) \in W$ with

$$f_W(\tau) = \frac{L_w \theta}{L_x} (e^{L_x \tau} - 1) \tag{11}$$

Proposition 2. (cf. Refs. 3 and 42). Consider the Lyapunov function $V(\cdot)$ of the nominal system of Eq. 1 under the controller h(x). There exists a quadratic function $f_V(\cdot)$ such that

$$V(x) \le V(\hat{x}) + f_V(|x - \hat{x}|)$$
 (12)

for all $x, \hat{x} \in \Omega_{\rho}$ with

$$f_V(s) = \alpha_4(\alpha_1^{-1}(\rho))s + M_v s^2$$
(13)

where M_v is a positive constant.

Theorem 1. (cf. Ref. 3). Consider the system of Eq. 1 in closed-loop under the LEMPC design of Eq. 8 based on a controller h(x) that satisfies the conditions of Eq. 2. Let $\epsilon_w > 0$, $\Delta > 0$, $\rho > \rho_e \ge \rho_{\min} \ge \rho_s > 0$ satisfy

$$\rho_e \le \rho - f_V(f_W(\Delta)) \tag{14}$$

and

$$-\alpha_{3}(\alpha_{2}^{-1}(\rho_{s})) + L'_{x}M\Delta + L'_{w}\theta \leq -\epsilon_{w}/\Delta$$
(15)

If $x(t_0) \in \Omega_{\rho}$ and $N \ge 1$ where

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$$\rho_{\min} = \max\left\{ V(x(t+\Delta)) : V(x(t)) \le \rho_s \right\}$$
(16)

then the state x(t) of the closed-loop system is always bounded in Ω_{ρ} and is ultimately bounded in $\Omega_{\rho_{\min}}$.

Proof. In this proof, we examine feasibility and closedloop stability of the LEMPC of Eq. 8 for operation around one steady-state corresponding to one set of desired values of the scheduled states.

We first discuss the feasibility of the LEMPC of Eq. 8. This LEMPC is guaranteed to be feasible at all times if the state is maintained in Ω_{ρ} , as will be subsequently shown, because the Lyapunov-based control law implemented in sample-and-hold is a feasible solution (i.e., $u=h(x(t_k)), t \in [t_k, t_{k+1})$ and $u=h(\tilde{x}(t_j)), t \in [t_j, t_{j+1}), j=k+1, \ldots, k+N-1$, is always a feasible solution). The use of both the Mode 1 and Mode 2 constraints at once poses no feasibility issues, because the Lyapunov-based controller implemented in sample-and-hold is a feasible solution to both constraints. This feasibility, however, is only ensured when the initial value of the state at the time t_0 at which the LEMPC of Eq. 8 first begins to be used is within Ω_{ρ} because the Lyapunov-based controller h(x) implemented in sample-and-hold is only guaranteed to maintain closed-loop stability of states within Ω_{ρ} .

Closed-loop stability is guaranteed at all times by the LEMPC formulation of Eq. 8. Before t', the state is always guaranteed to be within Ω_{ρ} from the use of the Mode 1 and Mode 2 constraints when the state leaves Ω_{ρ_e} using the same proof as in Ref. 3. The requirement that the contractive constraint be enforced whenever $|x_i(t_k)| \ge \gamma_i$ ensures that the Lyapunov function of the closed-loop state decreases whenever the state leaves this bound, which ensures that the state can always be driven back into a region where this bound is met in finite time. Furthermore, the contractive constraint always forces the state to $\Omega_{\rho_{\min}}$, so after t', it is guaranteed to be driven into this small region containing the origin.

The fact that feasibility of the LEMPC design of Eq. 8 hinges on whether $x(t_0) \in \Omega_\rho$ shows that when there is a plan to switch the production level to the next that is required in the schedule and thus to adjust the V, Ω_{ρ_a} , Ω_{ρ} , h(x), f, and origin used in Eq. 8, the state at the time t_1 at which the LEMPC is reformulated for the new production level in the schedule must be within the stability region of the new steadystate. In general, it is difficult to characterize the points that may be accessed by the closed-loop state under LEMPC within Ω_{ρ} without extensive closed-loop simulations from various initial conditions. The only region within the stability region of the first steady-state in which it is guaranteed that a process can be forced to operate is $\Omega_{
ho_{\min}}$, such that if the state is always driven into this region first and the new stability region overlaps this region, it can be guaranteed that a feasible solution to the new problem will exist. Another advantage of including $\Omega_{\rho_{\min}}$ within the overlap of the level sets is that any prior scheduled value of the state can be requested in the future and can be reached, since each stability region includes both $\Omega_{\rho_{\min}}$ of the set-point that it is designed with respect to, and also that of at least one other production level in the schedule. This motivates the following theorem, which characterizes the conditions under which the LEMPC formulation of Eq. 8 can be updated to drive the state to new values of the scheduled states without losing controller feasibility at t_1 , both when t_s is known *a priori* and when it is not. In this theorem, the time length t_h is defined as an upper bound on the worstcase time to drive the closed-loop state from any initial condition in the stability region into $\Omega_{\rho_{\min}}$ using the LEMPC (Mode 2 operation). Although the actual worst-case time to drive the closed-loop state from any initial condition in Ω_{ρ} into $\Omega_{\rho_{min}}$ is a closed-loop property (and thus cannot be evaluated based on the open-loop process dynamics alone), we will define a worst-case upper bound on this time to be t_h in the following theorem using the results from Ref. 3. Specifically, in the proof of Theorem 1 in Ref. 3, a worst-case upper bound $-\epsilon_w/$ Δ on \dot{V} under LEMPC is developed, where ϵ_w is a positive constant (defined in Theorem 1 above) related to the process dynamics, disturbance magnitude, sampling period, and Lyapunov-based controller properties. This bound is not necessarily tight, but it can allow the worst-case time t_h to be defined. To determine the time required to decrease V from its value for any initial condition in Ω_{ρ} to its value in $\Omega_{\rho_{\min}}$, the worst-case value $\dot{V} = -\epsilon_w / \Delta$ can be assumed. Then, this bound can be integrated from $V = \rho$ at $t_0 = 0$ to $V = \rho_{\min}$ at t. The result of solving for the time at which $V = \rho_{\min}$ assuming this worstcase rate is $t_h = \frac{-\Delta(\rho_{\min} - \rho)}{1}$. It is notable that from the proof of Theorem 1 in Ref. 3, the time t_h will also be a worst-case upper bound on the time required by a Lyapunov-based controller implemented in sample-and-hold to drive the closedloop state into $\Omega_{\rho_{\min}}$ from any initial condition in Ω_{ρ} .

Theorem 2. Consider the process of Eq. 1 operated under the LEMPC of Eq. 8 formulated with respect to a steadystate having stability region Ω_{ρ_1} with $\Omega_{\rho_{\min}} \subseteq \Omega_{\rho_1}$ where $\Omega_{\rho_{\min}}$ is defined as in Eq. 16 for the steady-state with stability region Ω_{ρ_1} . If also $\Omega_{\rho_{\min}} \subseteq \Omega_{\rho_2}$ and t_s is known a priori such that t' can be chosen as $t'=t_s-t_h$, then $x(t_s) \in \Omega_{\rho_{\min}}$ and the LEMPC of Eq. 8 formulated with respect to a steady-state having stability region Ω_{ρ_2} is feasible at $t_1=t_s$. If t_s is not known a priori, then if $t'=t_s$ and $t_1=t_s+t_h$ and $\Omega_{\rho_{\min}} \subseteq \Omega_{\rho_1}$ and also $\Omega_{\rho_{\min}} \subseteq \Omega_{\rho_2}, x(t_1) \in \Omega_{\rho_{\min}}$ and the LEMPC of Eq. 8 formulated with respect to a steady-state having stability region Ω_{ρ_2} is feasible at t_1 .

Proof. The proof of this theorem relies on many concepts from the proof of Theorem 1 above. Specifically, if t_s is known a priori and $t'=t_s-t_h$, then if the LEMPC were applied, the process state would be within $\Omega_{\rho_{\min}} \subseteq \Omega_{\rho_1} \cap \Omega_{\rho_2}$ by t_s , regardless of the location of the initial state in Ω_{ρ_1} from the definition of t_h . The Mode 2 constraint of Eq. 8f, when implemented repeatedly, ensures that the applied control action drives the closed-loop state into $\Omega_{\rho_{\min}}$ in a finite time. Thus, if the Mode 2 constraint begins to be implemented repeatedly at t', the closed-loop state under the LEMPC of Eq. 8 will enter $\Omega_{\rho_{\min}}$ by t_s and then since $x(t_s) \in \Omega_{\rho_2}$, from Theorem 1, the LEMPC for the next steady-state will be feasible at t_s . Using similar logic, if t_s is not known a priori but the Mode 2 constraint is applied repeatedly starting at $t'=t_s$, then by $t_1=t_s+t_h$, the closedloop state has entered $\Omega_{\rho_{\min}} \subseteq \Omega_{\rho_2}$, and the LEMPC for the next steady-state is then feasible by Theorem 1.

Remark 5. If the worst-case time t_h is difficult to assess using the bound in Ref. 3, an estimate of the time t_h can be obtained with closed-loop simulations under the Lyapunovbased controller using initial conditions throughout the stability (feasible) region of the LEMPC for schedule management, but this may not provide the true worst-case time since the LEMPC may take longer to drive the closed-loop

Table 1. Latameter values of the CSTI	Table	1.	Parameter	Values	of	the	CSTR
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$T_0 = 300 \text{ K}$	$F = 5.0 \text{ m}^3/\text{h}$
$V = 1.0 \text{ m}^3$	$E=5.0\times10^4$ kJ/kmol
$k_0 = 8.46 \times 10^6 \text{ m}^3/\text{h kmol}$	$\Delta H = -1.15 \times 10^4 \text{ kJ/kmol}$
$C_p = 0.231 \text{ kJ/kg K}$	R=8.314 kJ/kmol K
$\rho_L = 1000 \text{ kg/m}^3$	

state into $\Omega_{
ho_{\min}}$ than would the Lyapunov-based controller. The bound t_h bounds the time required to drive the closedloop system from any initial condition in Ω_{ρ} into $\Omega_{\rho_{\min}}$ under both the LEMPC and under h(x), but it does not state whether the time required to drive the closed-loop state from a given initial condition in $\Omega_
ho$ into $\Omega_{
ho_{\min}}$ will be less under LEMPC or under the Lyapunov-based controller. Because the results of Theorem 2 are based on a worst-case scenario, they are conservative. It is possible to require a less restrictive condition on the time at which the change in the LEMPC formulation to drive the closed-loop state toward the next production level required by the schedule occurs (e.g., that any time after t_s that process monitoring logic detects that the closed-loop state has entered $\Omega_{\rho_1} \cap \Omega_{\rho_2}$, the steady-state corresponding to a production level in the schedule is changed within the LEMPC). However, to make guarantees regarding the time at which the LEMPC can be adjusted to reflect the new production level without losing controller feasibility, more rigorous conditions like those in Theorem 2 are required.

Application to a Chemical Process Example

In this section, we provide a chemical engineering example to illustrate the application of the proposed EMPC with production schedule management. Specifically, a non-isothermal continuous stirred tank reactor (CSTR) where an irreversible second-order exothermic reaction takes place is considered. The reactor converts the reactant A to the product $B (A \rightarrow B)$. An inert solvent containing the reactant A with a concentration of C_{A0} is fed to the reactor at a feed temperature of T_0 . The CSTR is covered with a heating jacket that supplies or removes heat from the reactor at a heat rate Q. The reactor has a constant volume of V, and the volumetric flow rate of the entering and exiting streams is F. The liquid has a constant density of ρ_L and a heat capacity of C_p . The CSTR firstprinciples dynamic model derived from mass and energy balances for this process is of the following form:

$$\frac{dC_A}{dt} = \frac{F}{V}(C_{A0} - C_A) - k_0 e^{-E/RT} C_A^2$$
(17a)

$$\frac{dC_B}{dt} = k_0 e^{-E/RT} C_A^2 - \frac{F}{V} C_B \tag{17b}$$

$$\frac{dT}{dt} = \frac{F}{V}(T_0 - T) - \frac{\Delta H k_0}{\rho_L C_p} e^{-E/RT} C_A^2 + \frac{Q}{\rho_L C_p V}$$
(17c)

where C_A and C_B are the reactant and product concentrations. The temperature in the reactor is *T* and the reaction preexponential factor is k_0 . *E* and ΔH are the activation energy and the enthalpy of the reaction, respectively (process parameter values are listed in Table 1). The CSTR is operated around an open-loop asymptotically stable steady-state that occurs at $[C_{As} \ C_{Bs} \ T_s] = [1.22 \ \text{kmol/m}^3 \ 2.78 \ \text{kmol/m}^3 \ 438.0 \ \text{K}]$ which corresponds to an input vector of $[C_{A0s} Q_s] = [4.0 \text{ kmol/m}^3 0.0 \text{ kJ/h}].$

The inlet concentration C_{A0} and the heat supply/removal rate Q are the manipulated inputs which are upper and lower bounded by physical limitations on actuators as follows: 0.5 $\leq C_{A0} \leq 7.5 \text{ kmol/m}^3 \text{ and } -5.0 \times 10^5 \leq Q \leq 5.0 \times 10^5 \text{ kJ/h}.$ The CSTR state and input vectors in deviation variable form are defined as follows: $x^T = [C_A - C_{As} C_B - C_{Bs} T - T_s]$ and $u^T = [C_{A0} - C_{A0s} Q - Q_s]$. In the simulations below, the process model of Eq. 17 was integrated numerically using the explicit Euler method with an integration time step of $h_c = 10^{-4}$ h. The control objective of the LEMPC is to minimize the heat supply and removal rate while meeting a desired production schedule of the desired product B (we assume full state feedback in this example such that a measurement of the concentration of the product B is available at each sampling time, i.e., we assume that the concentration of the product B is a measured output of the process that is required to meet the schedule and is also a state variable). Therefore, the economic measure used as the LEMPC cost function is given by:

$$\frac{1}{(t_{k+N}-t_k)}\int_{t_k}^{t_{k+N}} [\alpha Q(\tau)^2 + \beta (C_B(\tau) - C_{B_{desired}})^2]d\tau \qquad (18)$$

where α and β are weighting constants. Owing to practical considerations, we consider that a limited amount of reactant material is available for a given operating period of $t_p = 1$ h. Therefore, the time-averaged concentration of reactant fed to the reactor over the operating period should satisfy the following material constraint:

$$\frac{1}{t_p} \int_0^{t_p} u_1(\tau) \ d\tau = 0.0 \ \text{kmol/m}^3.$$
(19)

To ensure closed-loop stability of the process considered, a Lyapunov-based controller is designed. In this example, only one stability region and Lyapunov-based controller, designed with respect to the open-loop asymptotically stable steadystate described above, was used, even when the steady-state corresponding to a production level in the schedule is changed within the LEMPC. As will be demonstrated below, there were no feasibility or closed-loop stability issues for the simulations performed, illustrating that the regions of attraction for the steady-states corresponding to the various production levels were overlapping and that the closed-loop state was maintained within each region of attraction for the steady-state corresponding to a given production level during the duration of production at that level. An estimate of the region of attraction can be obtained utilizing the Lyapunov function established under the Lyapunov-based controller. In this example, Eq. 17b indicates that the concentration of the desired product C_B is affected by the concentration of the reactant C_A and the temperature T but not vice versa. Since the inputs of the system affect the reactant concentration and temperature differential equations directly in Eq. 17a and Eq. 17c, the stability analysis of the closed-loop system can be established on the basis of the (C_A, T) subsystem. Therefore we define a reduced state vector as $\hat{x}^T = [C_A - C_{As} T - T_s]$. The Lyapunov-based controller design can be represented as a vector with two components: $h^T(\hat{x}) = [h_1(\hat{x}) \ h_2(\hat{x})]$. The inlet concentration control law $h_1(\hat{x})$ was set to its steady-state value $(h_1(\hat{x}) =$ 0.0 kmol/m^3) to meet the material constraint of Eq. 19. The stabilizing Lyapunov-based control law for the rate of heat input $h_2(\hat{x})$ is the following⁴³:

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Figure 3. Concentration of product *B* in time for the CSTR of Eq. 17 under the LEMPC of Eq. 8 (without the use of γ to activate Mode 2) with the material constraint of Eq. 19, following the production schedule with changes in the required value of C_B every 2 h.

$$h_{2}(\hat{x}) = \begin{cases} -\frac{L_{\hat{f}}V + \sqrt{L_{\hat{f}}V^{2} + L_{g}V^{4}}}{L_{g}V}, & \text{if } L_{g}V \neq 0 \\ 0, & \text{if } L_{g}V = 0 \end{cases}$$
(20)

 $L_{\tilde{f}}V$ and L_gV denote the Lie derivatives of the Lyapunov function $V(\hat{x})$ with respect to $\tilde{f}(\hat{x})$ and $g(\hat{x})$, respectively, where $\tilde{f}(\hat{x})$ signifies the terms in Eqs. 17a and 17c (in deviation form) not including the inputs, and $g(\hat{x})$ signifies the terms multiplying the inputs in those equations. A quadratic Lyapunov function of the form $V(\hat{x}) = \hat{x}^T P \hat{x}$ was used to characterize the stability region of the closed-loop system with the following positive definite *P* matrix:

$$P = \begin{bmatrix} 1060 & 22\\ 22 & 0.52 \end{bmatrix}$$
(21)

Extensive closed-loop simulations were conducted under the Lyapunov-based controller $h(\hat{x})$. Specifically, to verify that this Lyapunov-based controller was indeed asymptotically stabilizing for the nonlinear system when implemented continuously (which is required for defining the stability region by

Eq. 2), a region around the steady-state in state-space was discretized and then the value of the time-derivative of the Lyapunov function along the trajectories of Eqs. 17a and 17c under $h(\hat{x})$ was evaluated at each of the state-space points within the discretization. It was determined from these simulations that a region around the origin could indeed be found within which V is negative using this Lyapunov-based controller (i.e., the Lyapunov-based controller was shown to be asymptotically stabilizing), and a level set of the Lyapunov function within which V < 0 (based on the discretization) was selected as the stability region of the closed-loop system. The regions needed in designing stability constraints in the LEMPC were selected as Ω_{ρ} with $\rho = 368$ and $\Omega_{\rho_{e}}$ with ρ_e =340. In the simulation below, the LEMPC design had a sampling period of Δ =0.1 h and a prediction horizon of N = 10.

It is assumed that the production schedule requires a change in the concentration of the desired product C_B every 2 h (i.e., $C_{B_{desired}} = 3 \text{ kmol/m}^3$ for the first 2 h of operation, 1.5 kmol/m³ for the next two, then 2.5, 2.7, and 2 kmol/m³ for times between 4 and 6 h, 6 and 8 h, and 8 and 10 h, respectively). The proposed LEMPC scheme was applied to the CSTR



Figure 4. Input trajectories for the CSTR of Eq. 17 under the LEMPC of Eq. 8 (without the use of γ to activate Mode 2) with the material constraint of Eq. 19, following the production schedule with changes in the required value of C_B every 2 h.

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Figure 5. State trajectories for the CSTR of Eq. 17 under the LEMPC of Eq. 8 (without the use of γ to activate Mode 2) with the material constraint of Eq. 19, following the production schedule with changes in the required value of C_B every 2 h.

of Eq. 17 to produce C_B concentrations that meet the desired schedule. The CSTR was initiated from the steady-state and the LEMPC optimization problem at each sampling time was solved using the interior-point solver IPOPT.⁴⁴ The weighting coefficients in the objective function were chosen to be $\alpha = 1$ and $\beta = 10,000$ to balance the difference in magnitude between Q and $C_B - C_{B_{desired}}$. Because it was found that the objective function drove the value of C_B to the scheduled value without the need to impose the Mode 2 constraint, the condition $|C_B - C_{B_{desired}}| \geq \gamma$ was not utilized in the LEMPC. The resulting concentration of the output (C_B) is presented in Figure 3, which demonstrates the ability of the proposed scheme to achieve the desired production schedule while taking into account allowable trajectories from the process dynamics.

The closed-loop input trajectories for the CSTR under the LEMPC throughout the 10 h of operation are presented in Figure 4. The trajectories show that the inputs were able to meet the material constraint while driving the value of C_B to $C_{B_{desired}}$. They also show that the use of heating (*Q*) was effectively minimized as required by Eq. 18, with u_2 remaining at low values for the majority of the time of operation. The trajectories of the reactant concentration and reactor temperature in deviations from the steady-state values ($C_A - C_{As}, T - T_s$) are presented in Figure 5. This figure shows that *T* and C_A evolved in a time-varying fashion, even after C_B reached $C_{B_{desired}}$, to maintain C_B at its required value while meeting the material constraint and minimizing the objective function.

To present the ability of this scheme to maintain the process within the stability region, the state-space trajectories of the reactant concentration and reactor temperature in deviations from the steady-state values $(C_A - C_{As}, T - T_s)$ are presented in Figure 6. The Lyapunov function values throughout the 10 h of operation are presented in Figure 7.

The simulations discussed above manipulated two inputs while maintaining the time-averaged inlet concentration at its steady-state value. The traditional approach for achieving the desired production schedule, when the time-averaged inlet concentration is constrained to equal the steady-state value, is to fix the inlet concentration to its steady-state value C_{A0s} and manipulate the heat input to achieve the desired schedule. This can lead to using more heat to achieve the same desired schedule since the problem involves only one manipulated input. Using the same optimization problem formulation as in the simulations above (with the same objective function and starting conditions) except with u_1 set to C_{A0s} , the total heat used in producing the first schedule for the first 2 h was 1.1378×10^6 kJ. However, when both inputs are manipulated to achieve the desired schedule, as demonstrated in the simulations above, the total heat used for producing the first schedule for the first 2 h was 1.1176×10^6 kJ which requested 2% less heat usage. Even though the total amount of reactant fed to the reactor throughout the 2 h of operation was the same in both cases, allowing the inlet concentration to be manipulated in a time-varying manner introduces extra flexibility that was utilized by the EMPC to minimize the objective function even further. Introducing more flexibility by allowing more inputs to be manipulated in a time-varying manner and also optimizing economics with respect to a subset of the state vector can in general enhance the economic performance. Although for this example the increase in the number of manipulated inputs



Figure 6. The state-space profile for the closed-loop CSTR of Eq. 17 under the LEMPC of Eq. 8 (without the use of γ to activate Mode 2) with the material constraint of Eq. 19 following the production schedule for the 10 h operating period starting at $[C_A(0), T(0)] =$ [1.2 kmol/m³, 438 K].



Figure 7. The Lyapunov function value as a function of time for the closed-loop CSTR of Eq. 17 under the LEMPC of Eq. 8 (without the use of γ to activate Mode 2) with the material constraint of Eq. 19 starting at $[C_A(0), T(0)] = [1.2 \text{ kmol/m}^3, 438 \text{ K}]$ following the production schedule with changes in the required value of C_B every 2 h.

resulted in only 2% economic benefit, using an EMPC for schedule management with multiple manipulated inputs can present higher economic performance in plants involving many more states where the desired production schedule is requested only over a subset of the entire state vector.

In the simulation presented above, we only imposed the Mode 2 constraint if the closed-loop state exited Ω_{ρ_e} because, as demonstrated through the results in Figure 3, the high penalty on the deviation of the value of C_B from its steady-state value in the objective function (Eq. 18) was effective at driving the concentration of the product B to its scheduled value and maintaining it there with every change in the production level required by the schedule, without the need to utilize the Mode 2 constraint to enforce this tracking capability. In addition, there were no disturbances in this simulation to move the closed-loop state away from the schedule or out of Ω_{ρ_e} , so the Mode 2 constraint was never activated. To demonstrate the application of the Mode 2 constraint, another simulation that involved significant plant disturbances was considered. Specifically, we considered the case where the production schedule required a change in the concentration of the desired product C_B from $C_{B_{desired}} = 3 \text{ kmol/m}^3$ to 2.78 kmol/m³ for the next 3 h. The CSTR was initiated from $[C_{As} C_{Bs} T_s] = [1 \text{ kmol/m}^3 3 \text{ kmol/m}^3 468.37 \text{ K}]$ and no disturbances were imposed in the first hour of operation. After that, we implemented a constraint of the form of Eq. 8f requiring that the closed-loop state stay at the scheduled value of $C_B = 2.78 \text{ kmol/m}^3$, and that if it deviates from this value by more than 0.01 kmol/m³ (i.e., $\gamma = 0.01$), that the Mode 2 constraint should be activated to drive the closed-loop state back toward the schedule. A bounded disturbance vector $w^T = [w_1 \ w_2]$ w_3 was added to the right-hand side of Eq. 17 (stationary bounded Gaussian white noise with variances $\sigma_1 = 1 \text{ kmol/m}^3$, $\sigma_2 = 1 \text{ kmol/m}^3$, and $\sigma_3 = 40 \text{ K}$ with bounds $|w_1| \leq 1$, $|w_2| \leq 1$, and $|w_3| \leq 40$). Disturbances were added for the first 40 sampling periods of the second and third hours of operation which caused the concentration of C_B to be driven outside of the desired product quality in which case Mode 2 was activated to drive the concentration of C_B back inside $\gamma = 0.01$. The LEMPC was effective at maintaining C_B near the scheduled value of the state at all times as presented in Figure 8.

Remark 6. The LEMPC for schedule management is particularly beneficial when the economics-based term in the cost function does not have its minimum at a steady-state of the process (i.e., time-varying operation is more profitable than steadystate operation). In traditional tracking MPC's that are designed to drive the closed-loop state to a steady-state, a quadratic cost function is used. In this chemical process example, the cost function has a quadratic form, but the process is not operated at steady-state (Figure 5 shows that the unscheduled states evolve dynamically after C_B reaches the schedule), but in general nonquadratic stage costs can be utilized within EMPC, which distinguishes it from tracking MPC (see, e.g., Refs. 45 and 46 for examples of the implementation of EMPC's for the same chemical process utilized in the example in the present manuscript but for which the objective function is a non-quadratic function to be maximized).

Conclusion

In this work, the concept of improving process profit while meeting a schedule with EMPC for production schedule management was proposed for nonlinear systems in which some of the states are constrained to follow a certain desired production schedule. Several formulations of EMPC for schedule



Figure 8. Concentration of product *B* in time for the CSTR of Eq. 17 under the LEMPC of Eq. 8 with the material constraint of Eq. 19, following the desired production schedule of $C_B = 2.78 \text{ kmol/m}^3$ with $\gamma = 0.01$ subject to plant disturbances starting at t=1 h.

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management, with practical considerations, were discussed with a focus on LEMPC with a soft constraint for the schedule because for this formulation, sufficient conditions to guarantee closed-loop stability of a process and feasibility of the controller could be derived. A chemical process example demonstrated that the proposed approach can handle significant changes in the desired values of the scheduled states throughout time to achieve the requested production schedule while maintaining closed-loop stability.

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