Economic Model Predictive Control with Time-Varying Objective Function for Nonlinear Process Systems

Matthew Ellis
Dept. of Chemical and Biomolecular Engineering, University of California, Los Angeles, CA 90095

Panagiotis D. Christofides
Dept. of Chemical and Biomolecular Engineering, University of California, Los Angeles, CA 90095

Dept. of Electrical Engineering, University of California, Los Angeles, CA 90095

Economic model predictive control (EMPC) is a control scheme that combines real-time dynamic economic process optimization with the feedback properties of model predictive control (MPC) by replacing the quadratic cost function with a general economic cost function. Almost all the recent work on EMPC involves cost functions that are time invariant (do not explicitly account for time-varying process economics). In the present work, we focus on the development of a Lyapunov-based EMPC (LEMPC) scheme that is formulated with an explicitly time-varying economic cost function. First, the formulation of the proposed two-mode LEMPC is given. Second, closed-loop stability is proven through a theoretical treatment. Last, we demonstrate through extensive closed-loop simulations of a chemical process that the proposed LEMPC can achieve stability with time-varying economic cost as well as improve economic performance of the process over a conventional MPC scheme. © 2013 American Institute of Chemical Engineers *AIChE J*, 60: 507–519, 2014
Keywords: process control, optimization

Introduction

Within the chemical process industries, achieving optimal operating performance of chemical processes has traditionally relied on steady state or static optimization to compute new optimal operating set points (steady states) to address dynamic energy pricing, customer demand changes, and other time-varying economic considerations. This paradigm divides economic optimization of chemical processes into two layers. In the upper layer, called the real-time optimization (RTO) layer, economically optimal steady states are computed using steady state models of the process; see, for instance, Refs. 1 and 2. The operating steady states are sent down to the lower process control layer as set points or targets for the lower-layer controller(s) to guide the process to the optimal set points and maintain operation at the set points until the set points are updated by the upper layer. In the lower layer, model predictive control (MPC) has been widely implemented within the chemical process industries. MPC is a control framework that takes advantage of a dynamic model to predict the future state and outputs of a process to compute optimal control actions with respect to a cost function while accounting for process constraints. The standard cost function of an MPC scheme is a quadratic cost

that penalizes the deviation of states and inputs from their corresponding set points.

While the two-layer paradigm of RTO and MPC has been successfully deployed in many applications, optimal dynamic performance of process systems has remained an open topic for research as traditional RTO systems only address static or steady state optimization. Additionally, the models used in the RTO and MPC layers are often not consistent which may result in set points computed by the upper layer that are unreachable by the lower layer.[3] To this end, many researchers have explored alternatives to the traditional RTO/MPC framework within the context of other two-layer frameworks including replacing the steady state model with a dynamic model in the upper layer, called dynamic RTO,[4–7] studying the rate at which the upper layer should be resolved,[4,6] proposing an intermediate layer between the RTO and MPC layer, called steady state target optimization, to compute set points that are reachable in the lower layer,[8,9] and using nonlinear MPC to compute target states corresponding to the desired set point.[10]

As another way to address the drawbacks of traditional RTO/MPC frameworks, the two layers can be merged into one layer by replacing the quadratic cost function in MPC with a cost function that directly accounts for the economics of the process. The resulting economically optimal control scheme is referred to as economic MPC (EMPC). Several formulations have been proposed in the literature to address the critical challenge of formulating a stabilizing controller resulting from replacing the quadratic cost function with a

Correspondence concerning this article should be addressed to P. D. Christofides at pdc@seas.ucla.edu.

general cost function.[3,11–19] Some of the more recent work on EMPC includes Ref. 17 where two EMPC schemes are proposed for a catalytic distillation process: one EMPC formulated with a pure economics-based cost function and another economics-oriented tracking controller. Both controllers demonstrated improved performance over a conventional tracking controller. In Ref. 14, an adaptive EMPC scheme for uncertain nonlinear systems was developed. In Ref. 20, a Lyapunov-based EMPC (LEMPC) scheme was applied to a large-scale process network used in the production of vinyl acetate and the applicability of EMPC to large-scale process networks was discussed. In Ref. 18, the necessity of dissipativity for optimal steady state operation was discussed as well as a stability analysis for averagely constrained EMPC with terminal constraint was carried out.

For stability purposes, the aforementioned EMPC schemes, with provable stability properties, use a steady state to impose constraints in the EMPC optimization problem to ensure closed-loop stability in their formulations, for example, the terminal constant[3] and the Lyapunov-based constraint.[15] Moreover, almost all these EMPC schemes are formulated with time-invariant economic cost functions. The limited work on EMPC with explicitly time-dependent cost functions includes replacing the traditional RTO system in existing industrial two-layer architecture with an EMPC formulated with a time-dependent cost function[21] and formulating an EMPC with a terminal constraint that enforces convergence of the predicted state to an equilibrium manifold instead of formulating the terminal constraint with the economically optimal steady state.[12] However, when the time scale of the time-varying economic information is comparable to the time scale of the process dynamics, economically optimal time-varying operation may not necessarily be at or even near the economically optimal steady state. Furthermore, most of the previous EMPC work has addressed nominal asymptotic stability of an equilibrium point of the closed-loop system and not closed-loop stability in the sense of boundedness of the state in a compact set. As a result, formulating a one-layer EMPC scheme with a time-dependent cost function that can operate the system in a dynamic and economically optimal fashion while maintaining the state in a bounded region in the presence of disturbances is an important and open research topic.

In the present work, an LEMPC scheme is developed that can accommodate an explicitly time-varying economic cost function. First, the formulation of the LEMPC scheme is presented. With this formulation, dynamic process economic optimization and process control are completely handled in a one-layer control structure which removes the need for an RTO layer. Second, closed-loop stability, in the sense of boundedness of the closed-loop state, is proven through a theoretical treatment of the LEMPC scheme. No restrictions on the type of economic cost function are required for provable closed-loop stability under the proposed LEMPC scheme. Last, the LEMPC is applied to a chemical process example to demonstrate through extensive closed-loop simulations that the proposed LEMPC achieves stability with time-varying economic cost arising due to variable energy pricing and product demand changes and results in improved closed-loop economic performance over a conventional RTO/MPC scheme (i.e., steady state operation).

Preliminaries

Notation

The notation $|\cdot|$ denotes the Euclidean norm of a vector and the notation $|\cdot|_Q$ denotes the weighted Euclidean norm of a vector (i.e., $|x|_Q^2 = x^T Q x$ where Q is a positive definite matrix). A scalar valued function $\alpha : [0, a) \to [0, \infty)$ is said to belong to class $\mathcal{K}$ if it is continuous, strictly increasing, and satisfies $\alpha(0) = 0$. The symbol $\Omega_{\rho(x_s)}$, where $x_s \in \Gamma \subset \mathbb{R}^n$, is a fixed parameter denotes a level set of a function $V(x, x_s)$ (i.e., $\Omega_{\rho(x_s)} = \{x \in \mathbb{R}^n | V(x, x_s) \leq \rho(x_s)\}$). The notation $\text{diag}(v)$ denotes a matrix whose diagonal elements are the elements of vector v and all the other elements are zeros.

Class of nonlinear systems

The following class of continuous-time nonlinear dynamic systems that can be written in the following state-space form is considered

$$\dot{x}(t) = f(x(t), u(t), w(t)) \tag{1}$$

where $x(t) \in \mathbb{R}^n$ denotes the state vector $u(t) \in U \subset \mathbb{R}^m$ denotes the manipulated input vector, and $w(t) \in W \subset \mathbb{R}^l$ denotes the disturbance vector. The vector field $f : \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^l \to \mathbb{R}^n$ is assumed to be a locally Lipschitz vector function of its arguments. The set of available control energy U is assumed to be the convex set

$$U = \{u \in \mathbb{R}^m | u_i^{\min} \leq u_i \leq u_i^{\max}, i = 1, \ldots, m\} \tag{2}$$

and the disturbance vector is assumed to be bounded in the following set

$$W = \{w \in \mathbb{R}^l | |w| \leq w_p\} \tag{3}$$

where w_p is some positive constant that bounds the norm of the disturbance vector. State measurements are assumed to be available and sampled synchronously at each time instance of the time sequence: $\{t_{k \geq 0}\}$ where $t_k = t_0 + k\Delta$, $k \in \mathbb{Z}^+$ and Δ is the sampling period. As a consequence of the discrete time sampling of the state, control actions are applied to the continuous-time system of Eq. 1 in a sample-and-hold fashion with sampling period Δ. The existence of an equilibrium manifold, which denoted as $\Gamma = \{x_s \in \mathbb{R}^n | \exists u_s \in U \text{s.t.} f(x_s, u_s, 0) = 0\} \subset \mathbb{R}^n$, is assumed for the system of Eq. 1. An additional assumption is made on the set Γ to ensure that the acceptable operating region is nonempty which is stated in the "Economic Model Predictive Controller with Time-varying Cost" section. For a given system, the equilibrium manifold Γ can be taken as the set of admissible operating steady states.

The economic cost of the system of Eq. 1 is assumed to have the following form

$$L_e(t, x(t), u(t)) \tag{4}$$

which depends explicitly on time. If the time scale of the change of the economic information is on a comparable time scale to the one of the process dynamics, the economically optimal strategy is to operate the process in a time-varying (transient) fashion while accounting for time-dependent process economics.[20] As a result, the class of chemical processes that may benefit from the EMPC methodology proposed in this work are processes in which the economic cost time variation is on a time scale comparable to the process dynamics.

Stabilizability assumption

A stabilizability assumption is imposed on the system of Eq. 1. For each fixed $x_s \in \Gamma$, the existence of an explicit Lyapunov-based controller $h(x, x_s)$ that renders x_s of the nominal system of Eq. 1 asymptotically stable under continuous implementation is assumed. Using converse theorems,[22,23] the existence of a Lyapunov function $V(x, x_s)$ follows from the stabilizability assumption. The Lyapunov function satisfies the following conditions

$$\alpha_1(|x-x_s|) \leq V(x,x_s) \leq \alpha_2(|x-x_s|) \tag{5a}$$

$$\frac{\partial V}{\partial x} f(x, h(x,x_s), 0) \leq -\alpha_3(|x-x_s|) \tag{5b}$$

$$\left| \frac{\partial V}{\partial x} \right| \leq \alpha_4(|x-x_s|) \tag{5c}$$

$$h(x,x_s) \in U \tag{5d}$$

for $(x-x_s) \in D$ and each $x_s \in \Gamma$ where D is an open neighborhood of the origin. For each $x_s \in \Gamma$, the stability region $\Omega_{\rho(x_s)}$ can be characterized for the closed-loop system of Eq. 1 with the explicit stabilizing controller $h(x, x_s)$. Numerous control laws that provide explicitly defined stability regions for the closed-loop system have been developed using Lyapunov techniques for various classes of nonlinear systems; see Refs. 24–26 and the references therein. The union of the stability regions is denoted as $\mathcal{X} = \bigcup_{x_s \in \Gamma} \Omega_{\rho(x_s)}$ and it is assumed to be a compact set.

By continuity and the local Lipschitz property assumed for the vector field f and taking into account that the manipulated inputs u are bounded and the continuous differentiable property of the Lyapunov function, there exists positive constants M, L_w, L_x, L_x', and L_w' such that

$$|f(x,u,w)| \leq M \tag{6}$$

$$|f(x,u,w) - f(x',u,0)| \leq L_x|x-x'| + L_w|w| \tag{7}$$

$$\left| \frac{\partial V(x,x_s)}{\partial x} f(x,u,w) - \frac{\partial V(x',x_s)}{\partial x} f(x',u,0) \right| \leq L_x'|x-x'| + L_w'|w| \tag{8}$$

for all $u \in U$, $w \in W$, and $x, x' \in \mathcal{X}$.

The union of the stability regions

A simple demonstration of the construction of the set $\mathcal{X}$ is provided to embellish the concept of the union set $\mathcal{X}$. The stability region of a closed-loop system under an explicit stabilizing control law can be estimated for a steady state in Γ through the off-line computation described below. After the stability regions of sufficiently many steady states in Γ are computed, the union of these sets can be described mathematically through various mathematical techniques (e.g., curve fitting, convex optimization, etc.). The basic algorithm is

1. For $j = 1$ to J (J is a sufficiently large positive integer).
1.1. Select a steady state $(x_{s,j})$ in the set Γ.
1.2. Partition state space near $x_{s,j}$ into I discrete points (I is a sufficiently large positive integer).
1.3. Initialize $\rho(x_{s,j}) := \infty$.
1.4. For $i = 1$ to I.
1.4.1. Compute $\dot{V}(x_i, x_{s,j})$. If $\dot{V}(x_i, x_{s,j}) > 0$, go to Step 1.4.2. Else, go to Step 1.4.3.
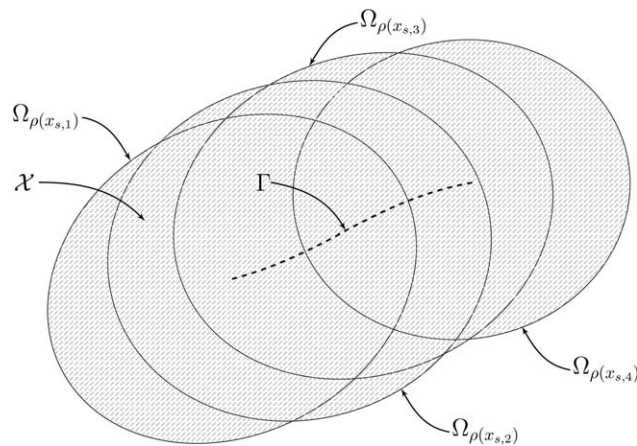1.4.2. If $V(x_i, x_{s,j}) \leq \rho(x_{s,j})$, set $\rho(x_{s,j}) := V(x_i, x_{s,j})$. Go to Step 1.4.3.

Figure 1. An illustration of the construction of the stability region $\mathcal{X}$.

1.4.3. If $i+1 \leq I$, go to Step 1.4.1 and $i \leftarrow i+1$. Else, go to Step 2.
2. Save $\rho(x_{s,j})$.
3. If $j+1 \leq J$, go to Step 1 and $j \leftarrow j+1$. Else, go to Step 4.
4. Approximate the union set with analytic mathematical expressions (constraints) using appropriate techniques.

If Γ consists of a finite number of points, then J could be taken as the number of points in Γ. If the number of points in Γ is large or infinite, J could be a sufficiently large integer. From a practical stand point, these numbers need to be small enough such that this type of calculation can be implemented. Figure 1 gives an illustration of the construction of $\mathcal{X}$ using this procedure. The following example provides a tractable illustration of the construction of $\mathcal{X}$ for a scalar system.

EXAMPLE 1. *Consider the nonlinear scalar system described by*

$$\dot{x} = x - 2x^2 + xu \tag{9}$$

with available control energy $u(t) \in [-100, 100]$ and with the set of admissible operating steady states defined as $\Gamma = \{x_s \in [-25, 25]\}$. The steady states in Γ are open-loop unstable. The system of Eq. 9 can be written in the following input-affine form

$$\dot{\bar{x}}(t) = f(\bar{x}(t)) + g(\bar{x}(t))\bar{u}(t) \tag{10}$$

where $\bar{x} = x - x_s$ and $\bar{u} = u - u_s$. For simplicity, consider a quadratic Lyapunov function of the form

$$V(x,x_s) = \frac{1}{2}(x-x_s)^2 \tag{11}$$

for the closed system of Eq. 9 under the following Lyapunov-based feedback control law[27]

$$\hat{h}(x,x_s) = \begin{cases} -\dfrac{L_f V + \sqrt{L_f V^2 + L_g V^4}}{L_g V} & \text{if } L_g V \neq 0 \\ 0 & \text{if } L_g V = 0 \end{cases} \tag{12}$$

where $L_f V$ and $L_g V$ are the Lie derivatives of the function V with respect to f and g, respectively. To account for the bound on the available control energy, the controller is formulated as

$$h(x, x_s) = 100 \, \text{sat}\left(\frac{\hat{h}(x, x_s)}{100}\right) \tag{13}$$

where sat $(\cdot)$ *denotes the standard saturation function.*

For this particular case, the stability region of the system of Eq. 9 with the stabilizing controller of Eq. 13 for the minimum and maximum steady state in the set Γ are used to approximate the set $\mathcal{X}$. For the steady state $x_{s,1} = -25$ with corresponding steady state input $u_{s,1} = -51$, the largest level set of the Lyapunov function where the Lyapunov function is decreasing along the state trajectory with respect to the steady state $x_{s,1}$ is $\Omega_{\rho(x_{s,1})} = \{x \in \mathbb{R} | V(x) \leq 300.25\}$, (i.e., $\rho(x_{s,1}) = 300.25$). For the steady state $x_{s,2} = 25$ and $u_{s,2} = 49$, the level set is $\Omega_{\rho(x_{s,2})} = \{x \in \mathbb{R} | V(x) \leq 2775.49\}$, (i.e., $\rho(x_{s,2}) = 2775.49$). Therefore, the union of the stability region is described as $\mathcal{X} = \{x \in [-49.5, 99.5]\}$.

Economic Model Predictive Controller with Time-varying Cost

In this section, the formulation, implementation strategy, and stability analysis of the proposed LEMPC which accounts directly for the time-varying economic cost function are given.

Formulation

First, consider the case where no disturbances and uncertainties affect the system of Eq. 1 (i.e., the nominal system of Eq. 1). As a direct consequence of the construction method used for $\mathcal{X}$, any state in $\mathcal{X}$ is also in a stability region of at least one acceptable operating steady state (i.e., any $x \in \mathcal{X}$ is also in $\Omega_{\rho(x_s)}$ for some $x_s \in \Gamma$). The stability properties of $\mathcal{X}$ make it an attractive choice to use in the formulation of a LEMPC. Namely, use $\mathcal{X}$ to formulate a constraint in the optimization problem of the LEMPC that allows the predicted state to evolve in a time-varying fashion while maintains the state in the bounded region $\mathcal{X}$. The existence of an input trajectory that satisfies the input constraint and that maintains operation in $\mathcal{X}$ is guaranteed because applying the input trajectory obtained from the Lyapunov-based controller with respect to the steady state x_s that the current state $x \in \Omega_{\rho(x_s)}$ is a feasible solution.

In any practical setting, process disturbances and uncertainties will affect the closed-loop system and the actual state trajectory will deviate from the predicted nominal trajectory. For this case, forcing the predicted state to be in $\mathcal{X}$ is not sufficient for maintaining the actual (time varying) state trajectory in $\mathcal{X}$ because the disturbances may force the system out of $\mathcal{X}$ over the sampling period and the input is applied in a sample-and-hold fashion to a continuous-time system. To make $\mathcal{X}$ an invariant set when operating the system in a time-varying fashion, a subset of $\mathcal{X}$ is defined and is denoted as $\hat{\mathcal{X}}$. The maximum size of this set is the largest subset of $\mathcal{X}$ such that for any state starting in $\hat{\mathcal{X}}$ forced outside of $\hat{\mathcal{X}}$ over one sampling period, the state trajectory will be maintained in $\mathcal{X}$ over the sampling period. The size of $\hat{\mathcal{X}}$ depends on the properties of the system and bound on the disturbance. Furthermore, any state $x(t_k) \in \mathcal{X} \backslash \hat{\mathcal{X}}$ can be forced back into the set $\hat{\mathcal{X}}$. This statement holds as a result of the method used to construct $\hat{\mathcal{X}}$ and $\mathcal{X}$. In other words, a steady state $\hat{x}_s \in \Gamma$ can be found such that the current state is in its stability region $\Omega_{\rho(\hat{x}_s)}$. Then, a Lyapunov-based constraint can be used in the formulation of the LEMPC to

ensure that the computed control action $u(t_k)$ decreases the Lyapunov function by at least the rate given by the explicit stabilizing controller $h(x, \hat{x}_s)$ over the first sampling period in the prediction horizon to enforce convergence of the state back to the set $\hat{\mathcal{X}}$.

Given the definitions of the sets $\mathcal{X}$ and $\hat{\mathcal{X}}$, a slight clarification must be made on the set Γ. First, the set Γ is the set of points in state space that satisfies the steady state process model equation for some $u_s \in U$ (i.e., $f(x_s, u_s, 0) = 0$). Second, the union of the stability regions $\Omega_{\rho(x_s)}$ constructed for each steady state in Γ must form a nonempty, compact set. As pointed out, the intersection of all these stability regions is defined as $\mathcal{X}$. Last, there must exist a nonempty set, $\hat{\mathcal{X}}$, satisfying $\Gamma \subseteq \hat{\mathcal{X}} \subset \mathcal{X}$ such that if $x(t_k) \in \hat{\mathcal{X}}$, then $x(t_{k+1}) \in \mathcal{X}$ for a given system and bounded disturbance. Usually, one possible choice of $\hat{\mathcal{X}}$ is to take it to be Γ as Γ would typically satisfy these properties. If this is not the case or if $\hat{\mathcal{X}}$ is empty, then the set Γ must be reduced to construct a set $\hat{\mathcal{X}}$ that is nonempty. The importance of constructing $\hat{\mathcal{X}}$ to be nonempty comes from the fact that the set $\hat{\mathcal{X}}$ is where the LEMPC is allowed to operate the system in a dynamically optimal fashion. From a stability perspective, the LEMPC would still work if $\hat{\mathcal{X}}$ is empty as the controller would always operate in mode 2.

Using the sets Γ, $\mathcal{X}$, and $\hat{\mathcal{X}}$, the proposed LEMPC formulation with an explicitly time-varying cost is given by the following optimization problem

$$\underset{u \in S(\Delta)}{\text{minimize}} \int_{t_k}^{t_{k+N}} L_e(\tau, \tilde{x}(\tau), u(\tau)) d\tau \tag{14a}$$

$$\text{subject to } \dot{\tilde{x}}(t) = f(\tilde{x}(t), u(t), 0) \tag{14b}$$

$$\tilde{x}(t_k) = x(t_k) \tag{14c}$$

$$u(t) \in U \quad \forall t \in [t_k, t_{k+N}) \tag{14d}$$

$$\hat{x}(t) \in \hat{\mathcal{X}} \quad \forall t \in [t_k, t_{k+N}) \text{ if } x(t_k) \in \hat{\mathcal{X}} \tag{14e}$$

$$\hat{x}(t) \in \mathcal{X} \quad \forall t \in [t_k, t_{k+N}) \text{ if } x(t_k) \in \mathcal{X} \backslash \hat{\mathcal{X}} \tag{14f}$$

$$\frac{\partial V(x, \hat{x}_s)}{\partial x} f(x(t_k), u(t_k), 0) \leq \frac{\partial V(x, \hat{x}_s)}{\partial x} f(x(t_k), h(x(t_k), \hat{x}_s), 0)$$

$$\text{if } x(t_k) \notin \hat{\mathcal{X}}, x(t_k) \in \Omega_{\rho(\hat{x}_s)} \text{ with } \hat{x}_s \in \Gamma \tag{14g}$$

where $S(\Delta)$ is the family of piecewise constant functions with sampling period Δ, N is the prediction horizon of the LEMPC, $L_e(\tau, x(\tau), u(\tau))$ is the explicitly time-dependent economic measure of Eq. 4 which defines the cost function of the optimization problem, $\tilde{x}(t)$ denotes the predicted state trajectory of the system with input trajectory $u(t)$, $t \in [t_k, t_{k+N}]$ computed by the LEMPC and $x(t_k)$ is the state measurement obtained at time t_k. The optimal solution of this optimization problem is denoted as $u^*(t|t_k)$ and it is defined for $t \in [t_k, t_{k+N})$.

In the optimization problem of Eq. 14, Eq. 14a defines the economic cost function to minimize over the prediction horizon. The constraint of Eq. 14b is the nominal model of the system ($w(t) \equiv 0$) used to predict the evolution of the system with input trajectory $u(t)$ computed by the LEMPC and an initial condition given in Eq. 14c obtained through state measurement feedback. The constraint of Eq. 14d is the bound on the available control energy. The constraint of Eq. 14e defines mode 1 operation of the LEMPC and is active when the state at the current sampling time $x(t_k) \in \hat{\mathcal{X}}$. It

enforces that the predicted state trajectory be maintained in $\hat{\mathcal{X}}$. The constraint of Eq. 14f is active when $x(t_k) \in \mathcal{X} \backslash \hat{\mathcal{X}}$ and ensures the predicted state be contained in the set $\mathcal{X}$. The constraint of Eq. 14g defines mode 2 operation of the LEMPC and is active when the state is outside $\hat{\mathcal{X}}$. It is used to force the state back into the $\hat{\mathcal{X}}$ which is guaranteed for any $x(t_k) \in \mathcal{X}$. Although Eq. 14f is not needed for stability, it is used to ensure that the LEMPC optimizes the input trajectory with knowledge that the future evolution must be contained in $\mathcal{X}$, and helps to improve the closed-loop economic performance when the LEMPC is operating under mode 2 operation. Figure 2 illustrates the sets and different operation modes of the closed-loop system under the LEMPC of Eq. 14.

Remark 1. The set $\hat{\mathcal{X}}$ does not necessarily need to be the largest subset of $\mathcal{X}$ where if $x(t_k) \in \hat{\mathcal{X}}$, then $x(t_{k+1}) \in \mathcal{X}$. This set could be taken as a smaller set. For instance, if it is desirable to maintain operation near the acceptable operating steady states, $\hat{\mathcal{X}}$ could be taken as Γ or a slightly larger set than Γ.

Implementation strategy

The LEMPC of Eq. 14 is implemented in a receding horizon fashion for robustness to disturbances and uncertainty. Namely, the optimization problem is resolved every sampling period Δ after receiving state feedback from the system. The implementation strategy can be summarized as follows:

1. At sampling time t_k, the LEMPC receives a state measurement $x(t_k)$ from the sensors.

2. If $x(t_k) \in \hat{\mathcal{X}}$, go to Step 2.1. Else, go to Step 2.2.

2.1. LEMPC operates in mode 1: the constraint of Eq. 14e is active and constraints of Eqs. 14f–14g are inactive, go to Step 3.

2.2. LEMPC operates in mode 2: the constraint of Eq. 14e is inactive and constraints of Eqs. 14f–14g are active, go to Step 2.3.

2.3. Using a lookup table, find a $\hat{x}_s \in \Gamma$ such that $x(t_k) \in \Omega_{\rho(\hat{x}_s)}$, go to Step 3.

3. The LEMPC computes the optimal input trajectory $u^*(t)$ for $t \in [t_k, t_{k+N})$, go to Step 4.

4. The LEMPC sends the control action computed for the first sampling period of the prediction horizon to the control actuators to apply to the system in a sample-and-hold fashion from t_k to t_{k+1}. Go to Step 5.

5. $k \leftarrow k+1$. Go to Step 1.

Remark 2. For systems that are open-loop stable or do not have input constraints, the sets $\mathcal{X}$ and $\hat{\mathcal{X}}$ may be large (practically the entire $\mathbb{R}^n$), and the implementation strategy of the LEMPC and definition of these sets greatly simplifies.

Remark 3. Regarding finding the steady state $\hat{x}_s$ when the LEMPC is operating in mode 2, it may be any steady state with $x(t_k) \in \Omega_{\rho(\hat{x}_s)}$ although ideally the steady state $\hat{x}_s$ would be in the direction of the vector field at the current state for economically optimal performance.

Stability analysis

In this subsection, Theorem 1 provides sufficient conditions for closed-loop stability, in the sense of boundedness of the closed-loop system state inside the set $\mathcal{X}$, under the proposed LEMPC of Eq. 14a for any initial condition $x(t_0) \in \mathcal{X}$.
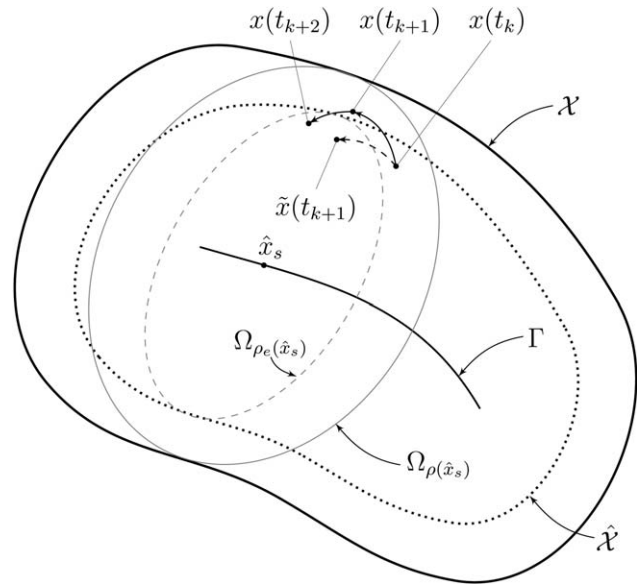

Figure 2. This illustration gives the state evolution over two sampling periods.

Over the first sampling period, the LEMPC, operating in mode 1, computes a control action that maintains the predicted state $\tilde{x}(t_{k+1})$ inside $\hat{\mathcal{X}}$. However, the actual state at the next sampling time $x(t_{k+1})$ is driven outside of $\hat{\mathcal{X}}$ by disturbances. The LEMPC, operating in mode 2, ensures that the computed control action decrease the Lyapunov function based on the steady state $\hat{x}_s$ over the next sampling period to force the state back into $\hat{\mathcal{X}}$.

Theorem 1 *Consider the system of Eq. 1 in closed-loop under the LEMPC design of Eq. 5 based on a controller $h(x, x_s)$ that satisfies the conditions of Eq. 5. Let $\epsilon_w > 0$, $\Delta > 0$, $\rho(x_s) > \rho_e(x_s) \geq \rho_{e,\min} > 0$ for all $x_s \in \Gamma$ satisfy*

$$0 < \rho_{e,\min} = \min_{x_s \in \Gamma} \{ \max \{ \rho_e(x_s) | \Omega_{\rho_e(x_s)} \subseteq \hat{\mathcal{X}} \} \} \quad (15)$$

and

$$-\alpha_3(\alpha_2^{-1}(\rho_{e,\min})) + L_x' M \Delta + L_w' w_p \leq -\epsilon_w / \Delta \quad (16)$$

If $x(t_0) \in \mathcal{X}$ and $N \geq 1$, then the state $x(t)$ of the closed-loop system is always bounded in $\mathcal{X}$.

Proof. The proof of Theorem 1 consists of the following parts: first, the feasibility of the optimization problem of Eq. 14 is proven for any state $x(t_k) \in \mathcal{X}$. Second, boundedness of the state trajectory $x(t) \in \mathcal{X}$ is proven for any initial state starting in $\mathcal{X}$.

Part 1. Owing to the construction of $\mathcal{X}$, any state $x(t_k) \in \mathcal{X}$ is also in the stability region $\Omega_{\rho(x_s)}$ of the controller $h(x, x_s)$ for some steady state x_s. This implies that there exists an input trajectory that is a feasible solution because the input trajectory $u(t_{k+j}) = h(x(t_{k+j}), x_s)$, $j = 0, 1, \ldots, N-1$ is a feasible solution to the optimization of Eq. 14a as it satisfies the constraints. The latter claim is guaranteed by the closed-loop stability properties of the Lyapunov-based controller $h(x, x_s)$. The reader may refer to Ref. 28 for a thorough discussion on the stability properties of the Lyapunov-based controller when implemented in a sample-and-hold fashion.

Part 2. If $x(t_k) \in \mathcal{X} \backslash \hat{\mathcal{X}}$, then the LEMPC operates in mode 2. As $x(t_k) \in \mathcal{X}$, a steady state $\hat{x}_s \in \Gamma$ can be found such that the current state $x(t_k) \in \Omega_{\rho(\hat{x}_s)}$ (recall $\Omega_{\rho(\hat{x}_s)}$ is computed from the Lyapunov-based controller $h(x, \hat{x}_s)$). Utilizing the Lyapunov-based controller $h(x, \hat{x}_s)$, the LEMPC computes control actions that satisfy the constraint of Eq. 14g

$$\frac{\partial V(x(t_k), \hat{x}_s)}{\partial x} f(x(t_k), u^*(t_k), 0)$$

$$\leq \frac{\partial V(x(t_k), \hat{x}_s)}{\partial x} f(x(t_k), h(x(t_k), \hat{x}_s), 0) \quad (17)$$

for some $\hat{x}_s \in \Gamma$ where $u^*(t_k)$ is the optimal control action computed by the LEMPC to be applied in a sample-and-hold fashion to the system of Eq. 1 for $t \in [t_k, t_{k+1})$. From Eq. 5b, the term in the right-hand side of the inequality of Eq. 17 can be upper bounded by a class $\mathcal{K}$ function as follows

$$\frac{\partial V(x(t_k), \hat{x}_s)}{\partial x} f(x(t_k), u^*(t_k), 0) \leq -\alpha_3(|x(t_k) - \hat{x}_s|) \quad (18)$$

The derivative of the Lyapunov function along the state trajectory for $\tau \in [t_k, t_{k+1})$ is

$$\dot{V}(x(\tau), \hat{x}_s) = \frac{\partial V(x(\tau), \hat{x}_s)}{\partial x} f(x(\tau), u^*(t_k), w(\tau)) \quad (19)$$

Adding and subtracting the term $\dot{V}(x(t_k), \hat{x}_s)$ to and from Eq. 19 and accounting for the bound of Eq. 18 and the Lipschitz properties of Eq. 8, the following bound can be derived that bounds the rate of decrease of the Lyapunov function due to the control action $u(t_k)$ and the rate of possible increase due to the disturbance $w(\tau)$ for $\tau \in [t_k, t_{k+1})$

$$\dot{V}(x(\tau), \hat{x}_s) \leq -\alpha_3(|x(t_k) - \hat{x}_s|) + L'_x|x(\tau) - x(t_k)| + L'_w|w(\tau)| \quad (20)$$

Utilizing Eq. 6 and the continuity of $x(t)$, the difference in the state over one sampling period can be bounded by

$$|x(\tau) - x(t_k)| \leq M\Delta \quad (21)$$

which holds for $\tau \in [t_k, t_{k+1})$ and M is a positive constant. Combining Eqs. 20 with 21 and accounting for the bound on the disturbance, the resulting bound on the time derivative of the Lyapunov function over one sampling period is

$$\dot{V}(x(\tau), \hat{x}_s) \leq -\alpha_3(|x(t_k) - \hat{x}_s|) + L'_x M\Delta + L'_w w_p \quad (22)$$

for all $\tau \in [t_k, t_{k+1})$.

As $x(t_k) \in \mathcal{X} \backslash \hat{\mathcal{X}}$ and $\Gamma \subseteq \hat{\mathcal{X}}$, the difference $|x(t_k) - \hat{x}_s|$ is always greater than zero. To upper bound the right-hand side of Eq. 22, a lower bound on the difference $|x(t_k) - \hat{x}_s|$ needs to be derived. Taking advantage of the level sets of $V(x, x_s)$, the largest level set $\Omega_{\rho_e(x_s)}$ contained in $\hat{\mathcal{X}}$ is computed for each $x_s \in \Gamma$ (refer to Figure 2 for an illustration of $\Omega_{\rho_e(\hat{x}_s)}$ for $\hat{x}_s$). Of all the level sets for each $x_s \in \Gamma$, the magnitude of the smallest level set denoted as $\rho_{e,\min}$ is used to bound the Lyapunov function value from below

$$V(x, \hat{x}_s) \geq \rho_{e,\min} \quad (23)$$

for all $x \in \mathcal{X} \backslash \hat{\mathcal{X}}$ and $\hat{x}_s \in \Gamma$ ($x \in \Omega_{\rho(\hat{x}_s)}$ and $\hat{x}_s \in \Gamma$; this is the condition of Eq. 15). Note also that $\rho_{e,\min} > 0$ as $|x(t_k) - \hat{x}_s| > 0$ for all $x \in \mathcal{X} \backslash \hat{\mathcal{X}}$ and $\hat{x}_s \in \Gamma$. Using the lower bound on the Lyapunov function of Eq. 23 and accounting for the bound of Eq. 5a, the difference $|x - \hat{x}_s|$ may be lower bounded by the following class $\mathcal{K}$ function

$$\alpha_2^{-1}(\rho_{e,\min}) \leq |x - \hat{x}_s| \quad (24)$$

which holds for all $x \in \mathcal{X} \backslash \hat{\mathcal{X}}$ and $\hat{x}_s \in \Gamma$. Applying this result to the bound on the time derivative of Eq. 22, the following bound is obtained

$$\dot{V}(x(\tau), \hat{x}_s) \leq -\alpha_3(\alpha_2^{-1}(\rho_{e,\min})) + L'_x M\Delta + L'_w w_p \quad (25)$$

for $x(t_k) \in \mathcal{X} \backslash \hat{\mathcal{X}}$. If the condition of Eq. 16 is satisfied, then there exists $\epsilon_w > 0$ such that the following inequality holds for $x(t_k) \in \mathcal{X} \backslash \hat{\mathcal{X}}$

$$\dot{V}(x(\tau)) \leq -\epsilon_w/\Delta, \ \forall \tau \in [t_k, t_{k+1}] \quad (26)$$

Integrating this bound on the interval $[t_k, t_{k+1})$, we obtain that

$$V(x(t_{k+1})) \leq V(x(t_k)) - \epsilon_w$$
$$V(x(\tau)) \leq V(x(t_k)), \ \forall \tau \in [t_k, t_{k+1}] \quad (27)$$

for all $x(t_k) \in \mathcal{X} \backslash \hat{\mathcal{X}}$. Using the above expression recursively, it follows that if $x(t_k) \in \mathcal{X} \backslash \hat{\mathcal{X}}$, then the state is driven closer to the equilibrium manifold Γ over each sampling time until it converges to $\hat{\mathcal{X}}$ as $\Gamma \subseteq \hat{\mathcal{X}}$. Furthermore, operation is always maintained within $\mathcal{X}$ because if $x(t_k) \in \hat{\mathcal{X}}$, then $x(t_{k+1}) \in \mathcal{X}$ owing to the construction of $\hat{\mathcal{X}}$ and if $x(t_k) \in \mathcal{X} \backslash \hat{\mathcal{X}}$, then $x(t_{k+1}) \in \mathcal{X}$. The latter fact holds because the state is forced to a smaller level set of the Lyapunov function with respect to the steady state $\hat{x}_s \in \Gamma$ over the sampling period. $\square$

Remark 4. Referring to Eq. 15, it is important to remark that it states to first select the largest level set (e.g., $\Omega_{\rho_e(x_s)}$) of $V(x, x_s)$ contained in $\hat{\mathcal{X}}$ for each steady state in the set Γ. From all these level sets, the smallest one denoted as $\Omega_{\rho_{e,\min}}$ is selected. Furthermore, it is important to point out that if $\Gamma = \{x_s^*\}$ (i.e., a set that only includes the optimal steady state), then the theoretical developments reduce to the previous work on LEMPC for time-invariant cost function; see Ref. 15. The sets $\mathcal{X}$ and $\hat{\mathcal{X}}$ would correspond to the sets Ω_ρ and $\Omega_{\hat{\rho}}$, respectively, in Ref. 15. Regarding the restrictions on the set of admissible steady states and the set $\hat{\mathcal{X}}$ that result from Eqs. 15 and 16, in order for these equations to hold the sampling period, bound on the disturbance, and the set $\hat{\mathcal{X}}$ must be sufficiently small as governed by Eqs. 15 and 16.

Remark 5. With the formulated constraints of the LEMPC of Eq. 14a, the optimization problem can always be made feasible regardless of whether the current state $x(t_k)$ is in $\mathcal{X}$ or not. For any state $x(t_k) \notin \mathcal{X}$, the Lyapunov-based constraint of mode 2 (Eq. 14g) can be formulated with any steady state in Γ (e.g., the steady state closest to the current state), and the controller would attempt to force the state closer to this steady state. While closed-loop stability (boundedness of the state) cannot be guaranteed for this case, it may still be possible for a state starting outside $\mathcal{X}$ to be forced into $\mathcal{X}$.

Remark 6. The two-mode control strategy of Eq. 14 parallels the LEMPC with time-invariant economic cost function that was first proposed in Ref. 15. For the LEMPC with time-invariant cost function, a subset of the stability region associated with the economically optimal steady state was found where the LEMPC was allowed to operate the system in a possibly time-varying fashion. The definition of this subset of the stability region could be clearly defined in terms of another level set of the Lyapunov function that depended on the sampling period, properties of the system, and bound on the disturbance. While similar type arguments could be used to derive a bound on $\hat{\mathcal{X}}$, this analysis has not been included in the present work because of the overly conservative nature of the result when applied to the LEMPC of Eq. 14.

Remark 7. No restriction on the form of the cost function is required for stability. However, some limitations to the cost function that can be considered must be made to solve the optimization problem. From a practical point-of-view, most, if not all, of the cost functions that would be used to describe the economics of a process system can be assumed to be piecewise continuous functions of time and sufficiently smooth functions with respect to the state and input vectors as they are typically derived from a total cost or profit which are generally not complex mathematical expressions.

Application to a Chemical Process Example

Consider a nonisothermal continuous stirred-tank reactor (CSTR) where three parallel reactions take place. The reactions are elementary irreversible exothermic reactions of the form: $A \rightarrow B$, $A \rightarrow C$, and $A \rightarrow D$. The desired product is B; whereas, C and D are byproducts. The feed of the reactor consists of the reactant A in an inert solvent and does not contain any of the products. Using first principles and standard modeling assumptions, a nonlinear dynamic model of the process is obtained

$$\frac{dC_A}{dt} = \frac{F}{V}(C_{A0}-C_A)-\sum_{i=1}^{3}k_{0,i}e^{-E_i/RT}C_A$$

$$\frac{dT}{dt} = \frac{F}{V}(T_0-T)-\frac{1}{\rho_R C_p}\sum_{i=1}^{3}\Delta H_i k_{0,i}e^{-E_i/RT}C_A+\frac{Q}{\rho_R C_p V}$$

(28)

where C_A is the concentration of the reactant A, T is the temperature of the reactor, Q is the rate of heat supplied or removed from the reactor, C_{A0} and T_0 are the reactor feed reactant concentration and temperature, respectively, F is a constant volumetric flow rate through the reactor, V is the constant liquid hold-up in reactor, ΔH_i, $k_{0,i}$, and E_i, $i=1,2,3$ denote the enthalpy changes, pre-exponential constants and activation energies of the three reactions, respectively, and C_p and ρ_R denote the heat capacity and the density of the fluid in the reactor. The process parameters are given in Table 1. The CSTR has two manipulated inputs: the inlet concentration C_{A0} with available control energy $0.5\text{kmol m}^{-3} \leq C_{A0} \leq 7.5\text{kmol m}^{-3}$ and the heat rate to/from the vessel Q with available control energy $-1.0\times10^5\text{kJ h}^{-1} \leq Q \leq 1.0\times10^5\text{kJ h}^{-1}$. The state vector is $x^T=[C_A\ T]$ and the input vector is $u^T=[C_{A0}\ Q]$.

Stability region construction

Supplying or removing significant amount of thermal energy to/from the reactor (nonzero Q) is considered to be undesirable from an economic perspective. Therefore, the set $\mathcal{X}$ is constructed considering steady states with a steady state reactant inlet concentration of $C_{A0s} \in [2.0, 6.0]\text{kmol m}^{-3}$ and no heat rate supplied/removed from the reactor (i.e., $Q_s=0.0\text{kJ h}^{-1}$). The corresponding steady states in the desired operating range form a set denoted as Γ of admissible operating steady states. Several of these steady states have been verified to be open-loop unstable (i.e., the eigenvalues of the linearization around the steady states corresponding to the minimum and maximum steady-state inlet concentrations are $\lambda_{1,\min}=-1.00$, $\lambda_{2,\min}=2.73$ and $\lambda_{1,\max}=-1.00$, $\lambda_{2,\max}=2.10$, respectively). The set Γ covers approximately a temperature range of 50 K.

Table 1. CSTR Process Parameters

Feedstock volumetric flow rate	$F=5.0\text{m}^3\text{h}^{-1}$
Feedstock temperature	$T_0=300\text{K}$
Reactor volume	$V=5.0\text{m}^3$
Pre-exponential factor for reaction 1	$k_{01}=6.0\times10^5\text{h}^{-1}$
Pre-exponential factor for reaction 2	$k_{02}=6.0\times10^4\text{h}^{-1}$
Pre-exponential factor for reaction 3	$k_{03}=6.0\times10^4\text{h}^{-1}$
Reaction enthalpy change for reaction 1	$\Delta H_1=-5.0\times10^4\text{kJ kmol}^{-1}$
Reaction enthalpy change for reaction 2	$\Delta H_2=-5.2\times10^4\text{kJ kmol}^{-1}$
Reaction enthalpy change for reaction 3	$\Delta H_3=-5.4\times10^4\text{kJ kmol}^{-1}$
Activation energy for reaction 1	$E_1=5.0\times10^4\text{kJ kmol}^{-1}$
Activation energy for reaction 2	$E_2=7.53\times10^4\text{kJ kmol}^{-1}$
Activation energy for reaction 3	$E_3=7.53\times10^4\text{kJ kmol}^{-1}$
Heat capacity	$C_p=0.231\text{kg m}^{-3}$
Density	$\rho_R=1000\text{kJ kg}^{-1}\text{K}^{-1}$
Gas constant	$R=8.314\text{kJ kmol}^{-1}\text{K}^{-1}$

A set of two proportional controllers is used in the design of the explicit stabilizing control law (i.e., the Lyapunov-based controller)

$$h(x,x_s)=\begin{cases} 3.5\ \text{sat}\left(\dfrac{K_1(x_{s,1}-x_1)+u_{1,s}-4.0}{3.5}\right)+4.0 \\ 10^5\ \text{sat}\left(\dfrac{K_2(x_{s,2}-x_2)+u_{2,s}}{10^5}\right) \end{cases}$$

(29)

where $K_1=10$ and $K_2=8000$ are the gains of each proportional controller. The proportional controllers have been tuned to give the largest estimate of the stability region for a given steady state. A quadratic Lyapunov function of the form

$$V(x,x_s)=(x-x_s)^T P(x-x_s)$$

(30)

where P is a positive definite matrix is used to estimate the stability regions of many steady states in the set Γ (i.e., the stability region is taken to be a level set of the Lyapunov function where the Lyapunov function is decreasing along the state trajectory; see the procedure outlined in the "Example Construction of the Union of Stability Regions" subsection). To obtain the largest estimate of the region $\mathcal{X}$, several different P matrices were used. The results of this procedure are shown in Figure 3. The union of these regions $\mathcal{X}$ was approximated with two quadratic polynomial inequalities and three linear state inequalities

$$1.26x_1^2-19.84x_1+467.66-x_2 \geq 0$$
$$2.36x_1^2-26.72x_1+428.26-x_2 \leq 0$$
$$0.4 \leq x_1 \leq 7.4$$
$$x_2 \leq 434.5$$

(31)

which will be used in the formulation of the LEMPC to ensure that the state trajectories are maintained inside $\mathcal{X}$.

Closed-loop simulation results

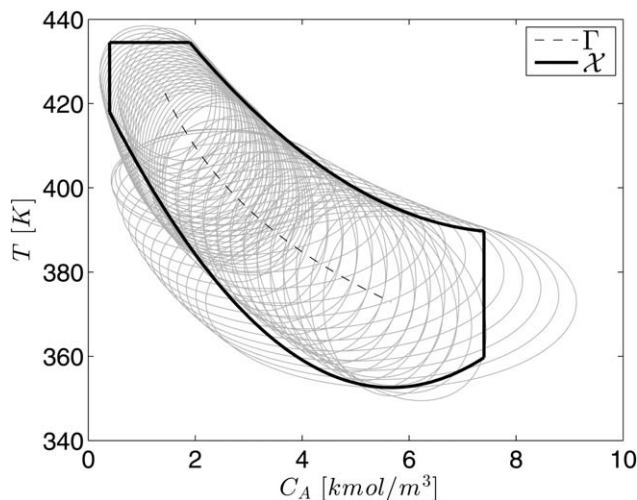The control objective of this chemical process example is to operate the CSTR in an economically optimal manner

Figure 3. The construction of the set $\mathcal{X}$ for the CSTR.

while accounting for changing economic factors and maintaining the system operation inside a bounded set. For this chemical process example, the economic measure being considered is

$$L_e(t,x,u)=A_1u_2^2+A_2u_1-A_3r_1(x)+A_4(x_2-395)^2 \quad (32)$$

where $r_1(x)$ is the reaction rate of the first reaction that produces the desired product

$$r_1(x)=k_{01}e^{-E_1/Rx_2}x_1 \quad (33)$$

The economic measure of Eq. 32 penalizes energy usage/removal, penalizes reactant material consumption, credits the production rate of the desired product, and penalizes the deviation of the operating temperature from the median operating temperature. The fourth term of the economic cost is used to prevent the LEMPC from operating the CSTR at the boundary of the allowable operating range for long periods of times which is considered undesirable from a practical perspective. In this fashion, the economic cost consists of terms that are associated with the operating cost (economic terms) as well as terms that ensure that the LEMPC operates the CSTR in a practical and safe fashion.

For this study, the weights A_1 and A_2 are considered to vary with time; while, $A_3=278$ and $A_4=0.4$ are constants over the 5.0 h simulated operation of the CSTR under the LEMPC. The weight A_1 is equal to 4.0×10^{-6} for $t=0.0-4.0$ h and 5.0×10^{-6} for 4.0–5.0 h, and the time-dependent weight A_2 is given by the following piecewise constant relationship

$$A_2=\begin{cases} 333 & 0.0h \leq t < 1.0h \\ 167 & 1.0h \leq t < 2.0h \\ 83 & 2.0h \leq t < 3.0h \\ 17 & 3.0h \leq t < 4.0h \\ 167 & 4.0h \leq t < 5.0h \end{cases} \quad (34)$$

As the economic cost is considered to account for more than just the operating cost (or profit) of the CSTR, the weights can be considered to account for more than the price of a particular resource. For instance, the variation of the weight A_2 may be caused by demand or supply changes of the reactant A from other processes within a single process-

ing facility. While these weights would come from a higher level information technology system, careful tuning of these weights is critical to achieve both practical operation with LEMPC as well as economically optimal (with respect to the actual operating cost) operation. For this particular study, the economic cost has been chosen to vary on a time scale comparable to the one of the process dynamics.

In the first set of simulations, nominal operation ($w(t) \equiv 0$) is considered to understand the operation of the CSTR under the LEMPC operating in mode 1 only. The formulation of the LEMPC with explicitly time-varying cost function used to accomplished the desired control objective is

$$\underset{u\in S(\Delta)}{\text{minimize}} \int_{t_k}^{t_{k+N}} L_e(\tau,\tilde{x}(\tau),u(\tau))d\tau$$

$$\text{subject to } \dot{\tilde{x}}(t)=f(\tilde{x}(t),u(t),0)$$

$$\tilde{x}(t_k)=x(t_k)$$

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

$$1.26x_1^2(t)-19.84x_1(t)+467.66-x_2(t) \geq 0 \quad \forall t \in [t_k,t_{k+N}]$$

$$2.36x_1^2(t)-26.72x_1(t)+428.26-x_2(t) \leq 0 \quad \forall t \in [t_k,t_{k+N}]$$

$$0.4 \leq x_1(t) \leq 7.4 \quad \forall t \in [t_k,t_{k+N}]$$

$$x_2(t) \leq 434.5 \quad \forall t \in [t_k,t_{k+N}]$$

$$(35)$$

where the economic measure L_e is given in Eq. 32. As no disturbances or uncertainties are present, the regions $\hat{\mathcal{X}}=\mathcal{X}$. The sampling period and the prediction horizon of the LEMPC is $\Delta=0.1$h and $N=10$, respectively. These parameters have been chosen through extensive simulations such that the total prediction horizon is sufficiently long to yield good economic performance of the closed-loop system. In other words, the LEMPC needs to observe enough of the future evolution of the system to make economically desirable decisions (with respect to the total length of operation of the CSTR) to optimally operate the CSTR in a time-varying fashion. To solve the LEMPC optimization problem at each sampling period, the open-source interior point solver Ipopt[29] was used. A fourth-order Runge-Kutta method with integration step of 5.0×10^{-4}h was used to numerically solve the nonlinear ODEs of Eq. 28. To assess the total economic performance of each simulation, the total economic measure over the simulated operation of the CSTR is defined as

$$\sum_{j=0}^{M}[A_1(t_j)u_2^2(t_j)+A_2(t_j)u_1(t_j)-A_3r_1(x(t_j))+A_4(x_2(t_j)-395)^2]$$

$$(36)$$

where M is the number of integration steps over the entire simulated time t_f.

Remark 8. While the nonlinear programming software Ipopt, which returns a local optimum, is used in this study to solve the LEMPC optimization problem, any other optimization software (e.g., a global optimization solver that can return the global optimum) can be used as long as it can return a solution to the optimization problem in considerably less time than the sampling time. However, if a global optimization solver is used, the time required to solve the optimization may significantly increase.[30]

The CSTR is initialized at the initial condition of $C_A(0)=2.0$kmol m^{-3} and $T(0)=410.0$K. As the exact future
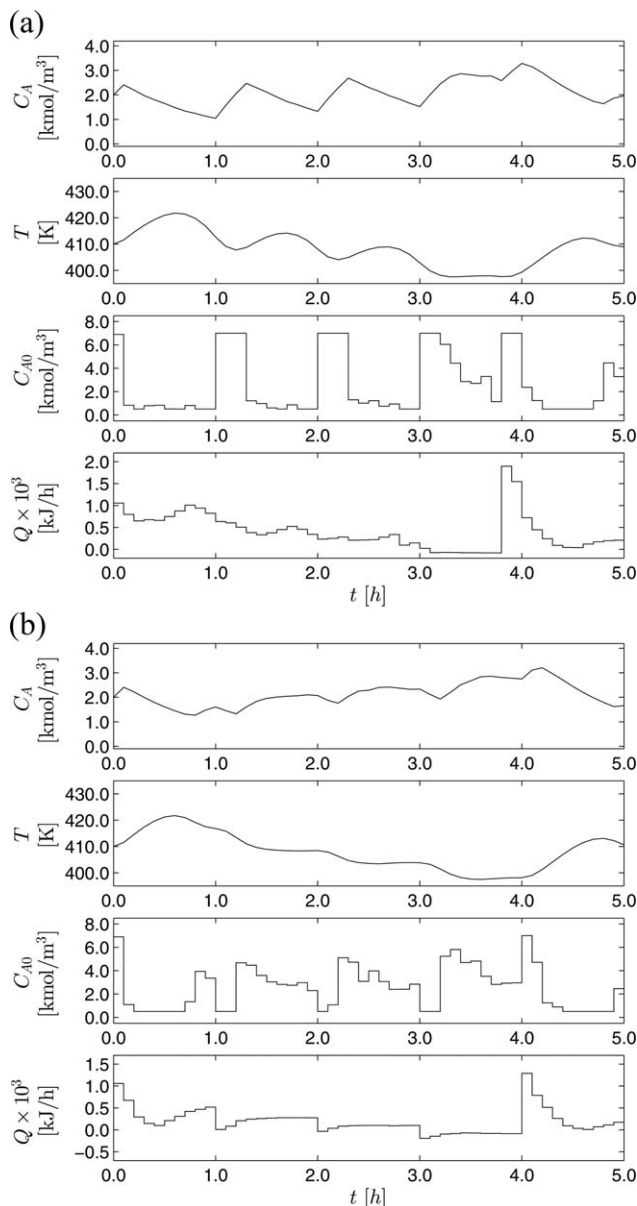
Figure 4. The states and inputs of the CSTR under nominal operation with the proposed LEMPC of Eq. 35 (i.e., mode 1 operation only) initialized at $C_A(0)=2.0$ kmol m^{-3} and $T(0)=410.0$K for (a) LEMPC-1 and (b) LEMPC-2.

values of the cost weights may not be known exactly in a practical setting, two cases were simulated: (1) the LEMPC knows the future cost weights $A_1(t)$ and $A_2(t)$ exactly which is denoted as LEMPC-1 and (2) the LEMPC only knows the cost weight values when the weights change which is denoted as LEMPC-2. For LEMPC-2, the previously obtained weights A_1 and A_2 are used in the optimization problem until the LEMPC receives new weight values which are obtained at the time instance the weights change. The results of these simulations are shown in Figure 4. Over the course of both of these simulations, the LEMPC schemes operate the CSTR in a time-varying (transient) fashion. If the economic weights become fixed or if a significant time-scale separation between economic cost change and the process dynamics existed, steady state operation would become optimal for this particular economic cost and nonlinear
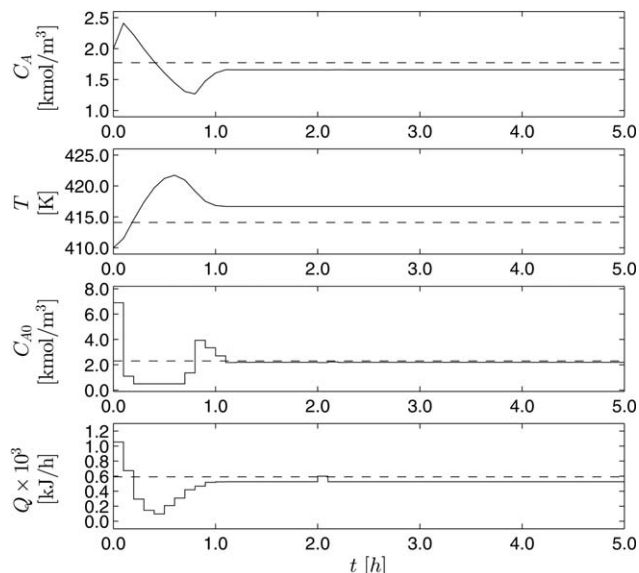

Figure 5. The states and inputs of the CSTR under the LEMPC of Eq. 35 (i.e., mode 1 operation only) when the economic cost weights are constant with time (solid line) with the economically optimal steady state (dashed line).

model. Also, the LEMPC in this example is not formulated with any periodic, average, or integral input constraints as in Refs. 11,15,16, and is not formulated with any stabilizing constraints to enforce convergence to the economically optimal steady state. Therefore, the reason for the time-varying operation is due to the economic cost changing with time on a time-scale comparable to the process dynamics. To demonstrate this point, Figure 5 shows the state and input trajectories under LEMPC of Eq. 35 (i.e., mode 1 only) where the economic cost weights are constant with time. Recalling the LEMPC does not have any constraints that enforce convergence to the steady state, the CSTR under the LEMPC with a prediction horizon of $N=10$ settles on a slightly offsetting steady state from the economically optimal steady state.

The total economic cost of the CSTR under LEMPC-1 is 2.37×10^4; whereas, the economic cost of the CSTR under LEMPC-2 is 2.91×10^4. The key factor that contributes to the performance degradation of the second simulation (as depicted in Figure 4) can be observed in the input trajectories that the two LEMPC schemes compute. For the LEMPC-1 simulation, the LEMPC knows that the cost of the reactant material decreases at the beginning of each of the first 4 h of operation so it waits to utilize this resource until the beginning of each of these hours when the price is less than in the previous hour. For the LEMPC-2 simulation, the LEMPC uses the minimum amount of reactant material at

Table 2. The Optimal Steady State with Respect to the Time-Varying Economic Weights

t	$C_{A,s}^*$	T_s^*	$C_{A0,s}^*$	Q_s^*
0.0h $\leq t <$ 1.0h	1.77	414.1	2.30	591.5
1.0h $\leq t <$ 2.0h	2.12	407.5	2.61	300.9
2.0h $\leq t <$ 3.0h	2.40	402.9	2.87	151.2
3.0h $\leq t <$ 4.0h	2.75	398.1	3.20	−80.0
4.0h $\leq t <$ 5.0h	2.12	407.5	2.61	240.6

Table 3. The Total Economic Cost over Several Simulations with Different Initial States

Initial State		Total Economic Cost ($\times 10^5$) and Improvement over Conventional MPC				
$x_1(0)$	$x_2(0)$	LMPC	LEMPC-1	Improvement	LEMPC-2	Improvement
2.0	410.0	0.908	0.237	73.9%	0.291	68.0%
2.0	425.0	2.325	0.456	80.4%	0.507	78.2%
4.0	370.0	4.274	1.234	71.1%	1.075	74.8%
4.0	395.0	2.744	0.152	94.4%	0.192	93.0%
5.0	370.0	4.164	0.634	84.8%	0.643	84.6%
6.0	360.0	5.370	1.375	74.4%	1.225	77.2%

The total economic cost of the simulations where the LEMPC knows the future cost weight values exactly is denoted as "LEMPC-1"; whereas, the simulations where the LEMPC does not know the future cost weights until the time they are updated to new values is denoted as "LEMPC-2."

the beginning of each of these 4 h. Also, the cost of the thermal energy Q increases over the last hour of the simulated operation. In the first case, the LEMPC utilizes the thermal energy before the price increases to increase the reactor temperature, and then, uses less energy thereafter. In the second case, the LEMPC supplies heat to the reactor when the cost of thermal energy has already increased. Comparing the evolution of the states in both cases, the regions of operation in state space between the two cases are similar.

Remark 9. If the future economic cost is not known, one may be able to find a method to decrease the performance degradation such as using the average value of the economic cost weights or using an estimate of the future weight values in the formulation of the LEMPC cost.

To assess the economic performance of the CSTR under the LEMPC, a comparison between the CSTR under the LEMPC and under a conventional RTO and MPC framework was carried out. The CSTR is simulated under a Lyapunov-based MPC (LMPC), formulated with a conventional quadratic cost; see Ref. 28 for details on LMPC, where the LMPC works to drive the system to the economically optimal steady state which is the minimizer of

$$\underset{(x_s,u_s)}{\text{minimize}} \, L_e(t, x_s, u_s)$$

$$\text{subject to } f(x_s, u_s, 0) = 0 \qquad (37)$$

$$u_s \in U, x_s \in \mathcal{X}$$

for a fixed t. The optimal steady state is denoted as $x_s^*(t)$ and the optimal steady state with time for the economic weights is given in Table 2.

The formulation of LMPC is as follows

$$\underset{u \in S(\Delta)}{\text{minimize}} \int_{t_k}^{t_{k+N}} \left(|\tilde{x}(\tau) - x_s^*(\tau)|_{Q_c} + |u(\tau) - u_s^*(\tau)|_{R_c} \right) d\tau$$

$$\text{subject to } \dot{\tilde{x}}(t) = f(\tilde{x}(t), u(t), 0)$$

$$\tilde{x}(t_k) = x(t_k)$$

$$u(t) \in U, \forall t \in [t_k, t_{k+N}) \qquad (38)$$

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

$$\leq \frac{\partial V(x(t_k), x_s^*(t_k))}{\partial x} f(x(t_k), h(x(t_k), x_s^*(t_k)), 0)$$

where the cost function is a conventional quadratic cost function that penalizes the deviation of states and inputs from the optimal (time varying) steady state. The Lyapunov-based constraint is similar to the mode 2 Lyapunov-based constraint (Eq. 14g) of the LEMPC. The sampling period

and prediction horizon of the LMPC are chosen to be the same as the LEMPC. The weighting matrices are $Q_c = \text{diag}([2788.00.6])$ and $R_c = \text{diag}([27.85.0 \times 10^{-7}])$. A quadratic Lyapunov function of the form given in Eq. 30 with a positive definite matrix $P = \text{diag}([280.09.0])$ is considered. The Lyapunov-based controller used in the formulation of the Lyapunov-based constraint is a set of P-controllers like in Eq. 29 with gains $K_1 = 1$ and $K_2 = 6000$. The P-controllers have been tuned less aggressively compared to the P-controllers used in the construction of the set $\mathcal{X}$ to allow the LMPC more freedom in the optimization of the control action.

The CSTR was initialized at several states in state space and was simulated with three control strategies: (1) the LEMPC-1, (2) the LEMPC-2, and (3) the LMPC that works to track the economically optimal steady state. The total economic cost of each simulation is given in Table 3. The operating trajectories of a simulation under LMPC is also given in Figure 6 to demonstrate the differences in achievable trajectories with the conventional MPC formulation working to track the economically optimal steady state. Clearly, the operating trajectories of the EMPC cannot be obtained by a conventional MPC, regardless of the tuning of the weighting matrices. From the results of Table 3, the economic performance of the system under both of the LEMPC schemes is better than the performance under the conventional LMPC.
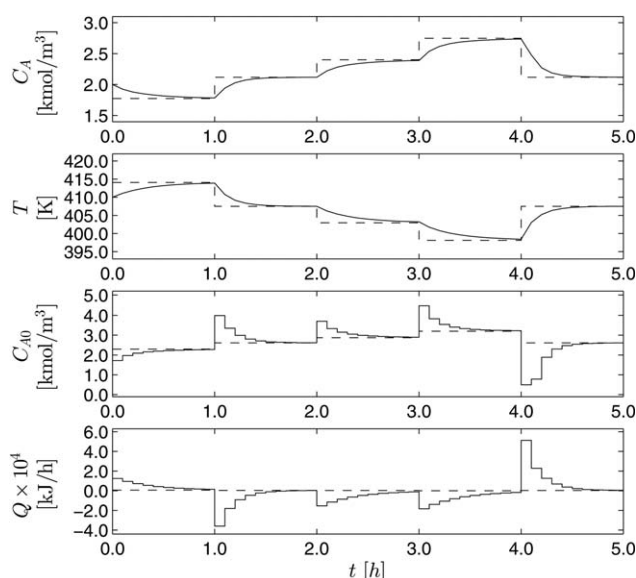

Figure 6. The states and inputs of the CSTR under the LMPC of Eq. 38 used to track the economically optimal steady state (dashed line).

For two of the initial conditions, the economic performance was better with LEMPC-2 compared to LEMPC-1 (Table 3). The closed-loop evolution of the CSTR with the two LEMPC schemes for one of these simulations is shown in Figure 7. In short, this is as a result of not having a sufficiently long prediction horizon for these two initial conditions. More specifically, this behavior is caused by initializing the CSTR far away from the economically optimal region to operate the process. For this prediction horizon ($N=10$), the LEMPC cannot simulate enough of the future evolution of the process to know there is an economically better region to operate the process. As a result, the state is maintained away from this optimal region at the beginning of both simulations. For the LEMPC-2 simulation, the maximum allowable amount of reactant concentration is fed to the process from 0.0 to 1.8 h. This causes the rates of the three reactions to increase. As the heat rate supplied/removed
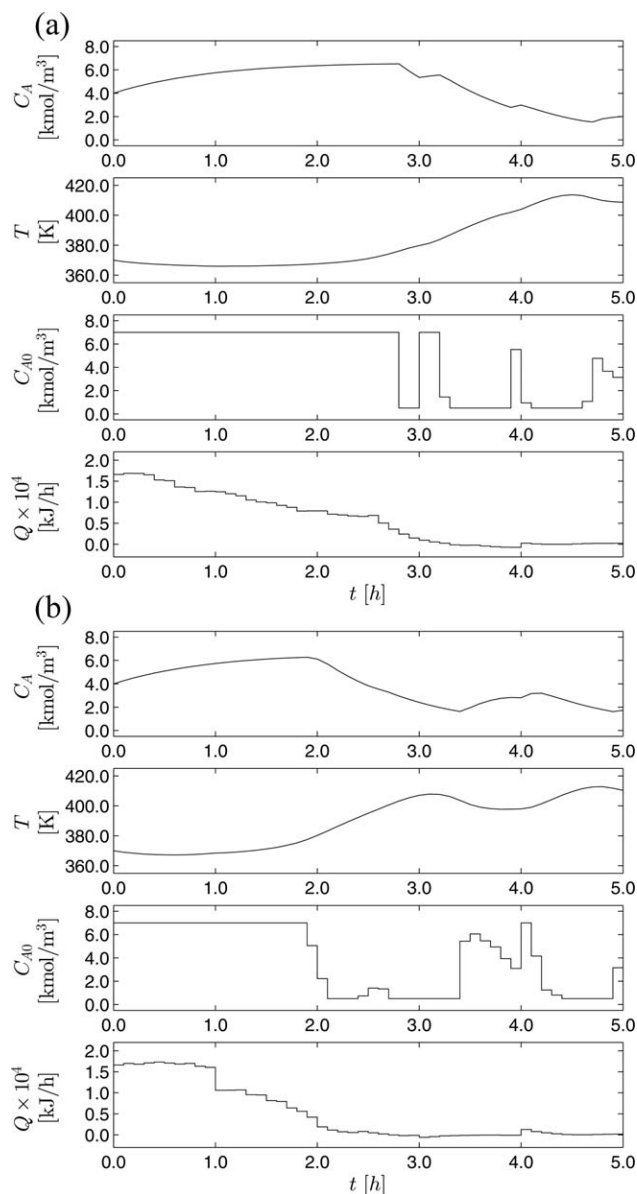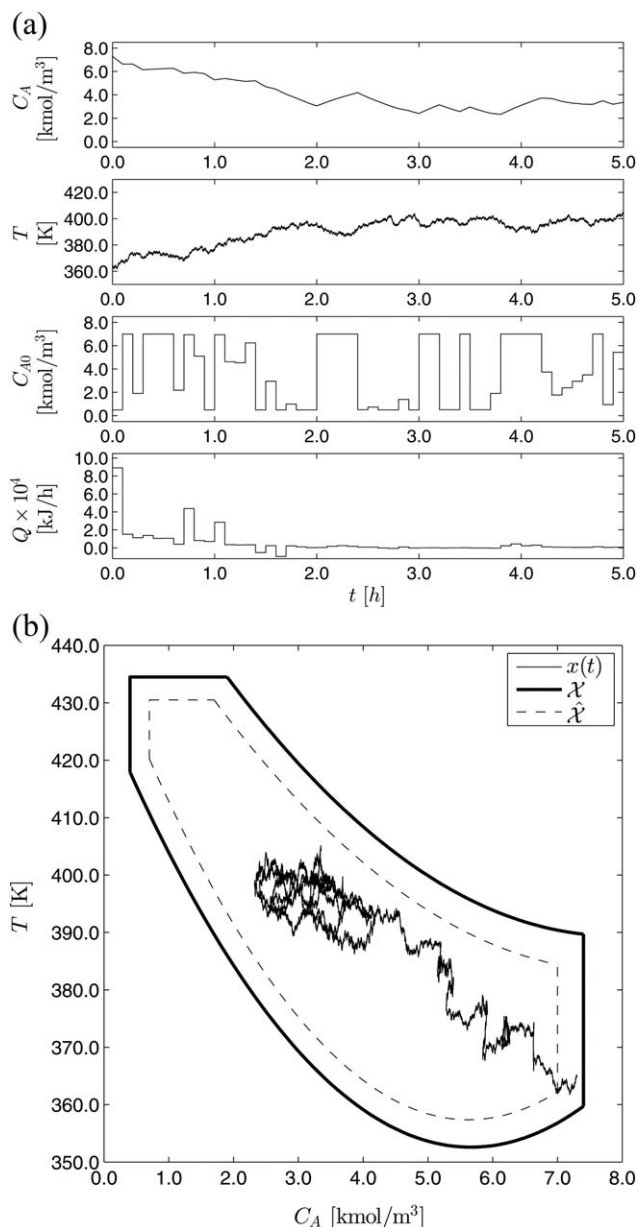
(a)

(b)

Figure 8. The states and inputs of the CSTR under the two-mode LEMPC with added process noise shown: (a) with time and (b) in state space.

from the reactor is penalized in the cost and the LEMPC does not know that the price of the reactant material will decrease at 2.0 h, Q and C_{A0} decrease leading up to 2.0 h to maintain stability. This decrease in Q and C_{A0} decreases the reactant concentration in the reactor while increasing the temperature bringing the states closer to the economically optimal region of operation. The LEMPC is then able to observe the economically optimal region of operation along its prediction horizon. Thus, it forces the states to this region. For LEMPC-1, the LEMPC knows that the reactant price will decrease at the beginning of each of the first 4 h. Therefore, it maintains feeding the maximum allowable reactant material to maximize reaction rate of the first reaction, and it supplies less heat to the reactor compared to LEMPC-2. As a result of this, operation is maintained far enough away from the economically optimal steady state such that the LEMPC cannot find the optimal region for operation.

Figure 7. The states and inputs of the CSTR under nominal operation with the proposed LEMPC of Eq. 35 initialized at $C_A(0)=4.0\,\mathrm{kmol\,m^{-3}}$ and $T(0)=370.0$K for (a) LEMPC-1 and (b) LEMPC-2.

Remark 10. Economic performance improvement under the LEMPC cannot be guaranteed in general. For guaranteed performance with a LEMPC scheme, refer to Ref. 31 which provides a method for guaranteed closed-loop performance improvement under LEMPC; this method can be extended to the case of time-varying cost using the set constraints $\hat{\mathcal{X}}$ and $\mathcal{X}$ with the performance constraints provided in Ref. 31. Specifically, to utilize the performance-based constraints, the LEMPC would need to be formulated with a shrinking horizon. The use of a shrinking horizon is covered in the stability analysis of this work as boundedness in $\mathcal{X}$ is proved for any horizon $N \geq 1$.

Remark 11. As it is difficult, for a general system and cost function, to determine the economically optimal region to dynamically operate a process, closed-loop simulations under EMPC must be carried out to determine this region. To ensure that the state converges to the economically optimal steady state, one could reduce the size of $\hat{\mathcal{X}}$ and enforce convergence to this set using a mode 2 type constraint in the LEMPC. Another way to address this problem is to use a sufficiently large horizon such that the LEMPC can explore enough state space to determine the economically optimal region of operation at the cost of increased computational burden.

To assess the stability and robustness properties of the proposed LEMPC, as discussed in the theoretical developments of the control framework, the size where the LEMPC is able to operate the system in a time-varying manner to optimize the process economic cost is reduced and the two-mode control strategy is used. Process noise is added to the closed-loop system and is modeled as bounded Gaussian white noise on the feed reactant concentration and temperature which has zero mean and the following standard deviation and bound: $\sigma_{C_{A0}} = 0.5 \, \text{kmol/m}^3$ and $w_{p,C_{A0}} = 1.0 \, \text{kmol/m}^3$ and $\sigma_{T_0} = 3.0 \text{K}$ and $w_{p,T_0} = 10.0 \text{K}$. To simulate the noise, a new random number is generated and used to add noise in the process model over each integration step. The region $\hat{\mathcal{X}}$ is approximated through the following constraints

$$
\begin{aligned}
1.20x_1^2 - 19.17x_1 + 460.61 - x_2 &\geq 0 \\
2.59x_1^2 - 29.14x_1 + 438.36 - x_2 &\leq 0 \\
0.7 \leq x_1 &\leq 7.1 \\
x_2 &\leq 431.5
\end{aligned}
\tag{39}
$$

which has been estimated through extensive simulations with the given process model, economic cost, and process noise as the region whereby closed-loop stability can be maintained. The results of a closed-loop simulation of the CSTR are displayed in Figure 8. The LEMPC does maintain the process inside the region $\mathcal{X}$ for the duration of the simulation as observed in Figure 8.

Conclusions

Accounting for dynamic energy costs and changing economic conditions is important for maximizing profit of a process. In this work, a LEMPC scheme that can handle dynamic economic conditions such as real-time changes in energy cost, demand, and feedstock pricing is presented. The formulation of the LEMPC scheme was provided as well as a rigorous theoretical treatment of the proposed control strategy. Closed-loop stability, in the sense of boundedness of the closed-loop state, under the proposed LEMPC was pro-

ven. A demonstration of the effectiveness of the LEMPC scheme on a chemical process example was provided. Compared to a conventional RTO/MPC scheme, the proposed LEMPC improved the closed-loop economic performance while maintaining stability of the process.

Literature Cited

1. Marlin TE, Hrymak AN. Real-time operations optimization of continuous processes. In: Proceedings of the Fifth International Conference on Chemical Process Control. AIChE Symposium Series, Tahoe City, CA, January 7–12, 1996;93:156–164.
2. Diehl M, Bock HG, Schlöder JP, Findeisen R, Nagy Z, Allgöwer F. Real-time optimization and nonlinear model predictive control of processes governed by differential-algebraic equations. *J Process Control*. 2002;12:577–585.
3. Rawlings JB, Bonné D, Jørgensen JB, Venkat AN, Jørgensen SB. Unreachable setpoints in model predictive control. *IEEE Trans Automat Control*. 2008;53:2209–2215.
4. Kadam JV, Schlegel M, Marquardt W, Tousain RL, van Hessem DH, van den Berg J, Bosgra O. A two-level strategy of integrated dynamic optimization and control of industrial processes—a case study. In: Grievink J, van Schijndel J, editors, Vol. 10. European Symposium on Computer Aided Process Engineering-12, Computer Aided Chemical Engineering. The Hague, The Netherlands: Elsevier, 2002:511–516.
5. Kadam JV, Marquardt W. Integration of economical optimization and control for intentionally transient process operation. In: Findeisen R, Allgöwer F, Biegler LT, editors. Vol. 358. Assessment and Future Directions of Nonlinear Model Predictive Control, Lecture Notes in Control and Information Sciences. Berlin Heidelberg: Springer, 2007:419–434.
6. Tosukhowong T, Lee JM, Lee JH, Lu J. An introduction to a dynamic plant-wide optimization strategy for an integrated plant. *Comput Chem Eng*. 2004;29:199–208.
7. Würth L, Hannemann R, Marquardt W. A two-layer architecture for economically optimal process control and operation. *J Process Control*. 2011;21:311–321.
8. Kassmann DE, Badgwell TA, Hawkins RB. Robust steady-state target calculation for model predictive control. *AIChE J*. 2000;46:1007–1024.
9. Muske KR. Steady-state target optimization in linear model predictive control. In: Proceedings of the 1997 American Control Conference, Albuquerque, NM, Vol. 6, 1997:3597–3601.
10. Huang R, Patwardhan SC, Biegler LT. Robust stability of nonlinear model predictive control with extended Kalman filter and target setting. *Int J Robust Nonlinear Control*. 2013;23:1240–1264.
11. Angeli D, Amrit R, Rawlings JB. On average performance and stability of economic model predictive control. *IEEE Trans Automat Control*. 2012;57:1615–1626.
12. Ferramosca A, Rawlings JB, Limon D, Camacho EF. Economic MPC for a changing economic criterion. In: Proceedings of the 49th IEEE Conference on Decision and Control (CDC), Atlanta, GA, 2010:6131–6136.
13. Grüne L. Economic receding horizon control without terminal constraints. *Automatica*. 2013;49:725–734.
14. Guay M, Adetola V. Adaptive economic optimising model predictive control of uncertain nonlinear systems. *Int J Control*. 2013;86:1425–1437.
15. Heidarinejad M, Liu J, Christofides PD. Economic model predictive control of nonlinear process systems using Lyapunov techniques. *AIChE J*. 2012;58:855–870.
16. Huang R, Harinath E, Biegler LT. Lyapunov stability of economically oriented NMPC for cyclic processes. *J Process Control*. 2011;21:501–509.
17. Idris EAN, Engell S. Economics-based NMPC strategies for the operation and control of a continuous catalytic distillation process. *J Process Control*. 2012;22:1832–1843.
18. Müller MA, Angeli D, Allgöwer F. On convergence of averagely constrained economic MPC and necessity of dissipativity for optimal steady-state operation. In: Proceedings of the 2013 American Control Conference (ACC). Washington, DC, 2013:3147–3152.

19. Rawlings JB, Angeli D, Bates CN. Fundamentals of economic model predictive control. In: 2012 IEEE 51st Annual Conference on Decision and Control (CDC). Maui, Hawaii, 2012:3851–3861.

20. Tu TS, Ellis M, Christofides PD. Model predictive control of a nonlinear large-scale process network used in the production of vinyl acetate. *Ind Eng Chem Res*. 2013;52:12463–12481.

21. Ellis M, Christofides PD. Integrating dynamic economic optimization and model predictive control for optimal operation of nonlinear process systems. *Control Engineering Pract*., in press, http://dx.doi.org/10.1016/j.conengprac.2013.02.016

22. Massera JL. Contributions to stability theory. *Ann Math*. 1956;64:182–206.

23. Khalil HK. *Nonlinear Systems*, 3rd ed. Upper Saddle River, NJ: Prentice Hall, 2002.

24. Kokotović P, Arcak M. Constructive nonlinear control: a historical perspective. *Automatica*. 2001;37:637–662.

25. Christofides PD, El-Farra NH. Control of Nonlinear and Hybrid Process Systems: Designs for Uncertainty, Constraints and Time-Delays. Berlin, Germany: Springer-Verlag, 2005.

26. Christofides PD, Liu J, Muñoz de la Peña D. Networked and Distributed Predictive Control: Methods and Nonlinear Process Network Applications. Advances in Industrial Control Series. London, England: Springer-Verlag, 2011.

27. Sontag ED. A "universal" construction of Artstein's theorem on nonlinear stabilization. *Syst Control Lett*. 1989;13:117–123.

28. Muñoz de la Peña D, Christofides PD. Lyapunov-based model predictive control of nonlinear systems subject to data losses. *IEEE Trans Automat Control*. 2008;53:2076–2089.

29. Wächter A, Biegler LT. On the implementation of an interior-point filter line-search algorithm for large-scale nonlinear programming. *Math Prog*. 2006;106:25–57.

30. Long CE, Polisetty PK, Gatzke EP. Nonlinear model predictive control using deterministic global optimization. *J Process Control*. 2006;16:635–643.

31. Heidarinejad M, Liu J, Christofides PD. Algorithms for improved fixed-time performance of Lyapunov-based economic model predictive control of nonlinear systems. *J Process Control*. 2013;23:404–414.