

# Optimal Time-varying Operation of Nonlinear Process Systems with Economic Model Predictive Control

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**ABSTRACT:** In the this work, we propose a two-layer approach to dynamic economic optimization and process control for optimal time-varying operation of nonlinear process systems. The upper layer, utilizing a Lyapunov-based economic model predictive control (LEMPC) system, is used to compute dynamic economic optimization policies for process operation. The lower layer, utilizing a Lyapunov-based MPC (LMPC) system, is used to ensure that the closed-loop system state follows the optimal time-varying trajectories computed by the upper layer over each finite-time operating window. To improve the computational efficiency of the two-layer structure, we allow both the LEMPC and the LMPC to compute control actions for two distinct sets of manipulated inputs thus decreasing the real-time computational demand compared to other one-layer EMPC schemes. Following a rigorous formulation and analysis of the proposed method, we demonstrate boundedness of the closed-loop system state and closed-loop economic performance improvement with the proposed two-layer framework compared to steady-state operation as well as with respect to other existing time-varying operating strategies previously proposed in the literature in the context of a benchmark chemical process application.

## ■ INTRODUCTION

Traditionally, the main objective of chemical process control systems is to ensure that chemical processes are operated at a steady-state. The operating steady-state may be changed depending on product grade changes and variable economic considerations. With this operation strategy in mind, a two-layer framework to process economic optimization and control is typically employed. The upper layer, called real-time optimization (RTO), computes an economically optimal steady-state using a steady-state process model. The computed steady-state is then sent down to the lower feedback control layer to steer the closed-loop system to the computed steady-state and to maintain operation at steady-state thereafter.<sup>1,2</sup>

While steady-state operation is typically used in chemical process industries, steady-state operation may not necessarily be the economically best operation strategy. As another way to operate a chemical process, time-varying or transient operation can improve economic process performance. Within the context of chemical process industries, the literature is rich with examples of chemical processes that demonstrate economic performance improvement with time-varying operation (see, for instance, refs 3 and 4 and references therein).

To this point, the literature on time-varying operation within process systems engineering has primarily focused on the economic performance improvement with periodic operation where an operating limit cycle is determined and the process is operated on this limit cycle. In ref 3, many examples of periodic operation were given which demonstrated that periodic forcing of concentration can yield activity improvements and better reactor performance for ammonia synthesis, sulfur dioxide oxidation, carbon monoxide oxidation, Claus reaction, methanol synthesis, multiple reaction systems, and polymerization reactions. In ref 4, examples of control of periodically operated reactors were given that include a more diverse set of manipulated variables that improve performance if periodically manipulated like feed temperature for catalytic packed bed reactors, coolant or heating fluid temperature for stirred tank reactors, and initiator flow rate or radiation intensity for stirred polymerization reactors. Periodic control strategies have also been studied in several other applications (see, for instance, refs 5-9). Other studies provided a more thorough discussion of specific instances where periodic operation can benefit reactor performance like the dynamic study of CO oxidation on supported platinum which demonstrated that periodic feed switching results in timeaveraged oxidation rates much greater than the maximum achievable by steady-state operation in ref 10 and the study of catalytic reactor networks where periodically switched inlet and outlet sections led to greater conversion in ref 11. Furthermore, some works have proposed techniques to help identify systems that can benefit from periodic operation and to determine the optimal periodic strategy to employ like the analytic procedure for determining the frequency response of a nonlinear chemical reactor model in ref 12, the generalized  $\Pi$ -criterion proposed in ref 13 to analyze the feasibility of periodic operation which was applied to continuously stirred tank reactor (CSTR) examples in ref 14, a numerical approach proposed for computing the effects of periodic input forcing by a shooting algorithm in ref 15, and the numerical method for determining optimal parameter values in forced periodic operation in ref 16.

While the periodic operating strategies listed above do demonstrate economic performance improvement, they are, in principle, ad hoc operating strategies and not necessarily optimal. Even periodic operating strategies that come from solving a

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dynamic optimization problem require that the switching pattern of the manipulated inputs be determined before solving the optimization problem as in ref 16. However, the periodic switching pattern determined before solving the optimization problem may not be optimal (i.e., the best time-varying operating strategy). Recent work has demonstrated how economic model predictive control (EMPC) can improve process performance through general time-varying operation to optimize a process economic measure (e.g., mode 1 operation of the Lyapunov-based EMPC (LEMPC) introduced in ref 17 and also refs 18-21 and references therein). The main advantage to EMPC is that it systematically determines the optimal operating strategy based on the economic measure in real time while accounting for state and input constraints and time-varying economic objectives and constraints. However, since EMPC oftentimes requires a larger prediction horizon for significantly improved closed-loop economic performance compared to conventional MPC (formulated with a quadratic cost function), it may be difficult to use EMPC to compute control actions for all the manipulated inputs of the system every sampling period because it requires solving a large-scale, potentially nonconvex optimization problem in real-time. For large-scale systems with many manipulated inputs and many states, this may be an impossible task.

While some techniques have been proposed to decrease the computational complexity of the EMPC such as a distributed EMPC framework for large-scale systems proposed in ref 22 and using singular perturbation theory when time-scale separation exists in the dynamics in ref 23 to formulate an EMPC on the basis of reduced-order models, the computational time EMPC requires still remains a challenge. We note that not all manipulated inputs may need to be computed by the EMPC to improve closed-loop performance significantly which was demonstrated in ref 23. Also, since many industrial applications have existing two-layer architectures for economic optimization and control (RTO and MPC), two-layer frameworks provide a natural and attractive method to decrease the computational demand of EMPC as pointed out in ref 24 where we proposed a two-layer architecture with EMPC in the upper layer and used a tracking LMPC to force the system to track the economically optimal operating trajectory over a finite-time operation period.

Motivated by the above, we propose a two-layer approach to dynamic economic optimization and process control for optimal time-varying operation of nonlinear process systems. The upper layer, utilizing a LEMPC system, is used to compute economically optimal policies for process operation and is solved only at the beginning of every operating window. The lower layer, utilizing a Lyapunov-based MPC (LMPC) system, is used to ensure the closed-loop system state follows the optimal time-varying trajectories computed by the upper layer over each finite-time operating window. To improve the computational efficiency of the two-layer structure, we allow both the LEMPC and the LMPC to compute control actions for two distinct sets of manipulated inputs thus decreasing the real-time computational demand compared to other one-layer EMPC schemes. Following a rigorous formulation and analysis of the proposed method, we demonstrate boundedness of the closed-loop system state and closed-loop economic performance improvement with the proposed two-layer framework compared to steady-state operation as well as with respect to other existing time-varying operating strategies previously proposed in the literature in the context of a benchmark chemical process application.

## PRELIMINARIES

**Notation.** The operator  $|\cdot|$  is used to denote the Euclidean norm of a vector and  $|\cdot|_Q$  denotes the weighted Euclidean norm of a vector (i.e.,  $|\cdot|_Q = x^T Q x$ ). A continuous function  $\alpha: [0,a) \rightarrow$  $[0,\infty)$  belongs to class  $\mathcal{K}$  functions if it is strictly increasing and satisfies  $\alpha(0) = 0$ . We use  $\Omega_{\rho}$  to denote the level set  $\Omega_{\rho} :=$  $\{x \in \mathbf{R}^n | V(x) \leq \rho\}$ . The symbol diag(v) denotes a square diagonal matrix with diagonal elements equal to the vector v.

**Class of Systems.** We consider a nonlinear process system described by the following state-space model:

$$\dot{x}(t) = f(x(t), u_1(t), u_2(t), w(t))$$
(1)

where  $x(t) \in \mathbf{R}^n$  denotes the state vector,  $u_1 \in U_1 \subset \mathbf{R}^{m_1}$  and  $u_2$  $\in U_2 \subset \mathbf{R}^{m_2}$  denotes two sets of manipulated inputs,  $w(t) \in \mathbf{R}^l$ denotes the disturbance vector, and f is assumed to be a locally Lipschitz vector function. The two sets of manipulated inputs are assumed to be bounded in nonempty convex sets:  $U_i :=$  $\{|u_{i,i}| \le u_{i,i}^{\max}: i = 1, ..., m_i\}$  for j = 1, 2. The two sets of manipulated inputs can also be viewed in terms of their main responsibilities. The inputs in set  $u_1$  are directly responsible for economic optimization and/or have the most significant impact on the process closed-loop economic performance, and the inputs in set  $u_2$  are responsible for maintaining closed-loop stability (see the Application to a Chemical Process Example section). The disturbance is assumed to be bounded, i.e.,  $W := \{w(t) \in$  $\mathbf{R}^{l}$ :  $|w(t)| \leq \theta$  where  $\theta$  is a positive parameter. The origin of the nominal unforced system of eq 1 is assumed to be an equilibrium point (i.e., f(0,0,0,0) = 0). We note in this work we propose a two-layer control framework and we assume without loss of generality that the state x of the system is sampled synchronously and the time instants at which we have state measurements are indicated by the time sequence  $\{t_{k>0}\}$  with  $t_k = t_0 + k\Delta$ , k = 0, 1, ... where  $t_0$  is the initial time, and  $\Delta = \Delta_1 = \Delta_2$ is the sampling time of both layers.

**Lyapunov-Based Controller.** We assume that there exists a Lyapunov-based controller

$$(u_1, u_2) = (h_1(x), h_2(x)) =: h(x)$$
(2)

which renders the origin of closed-loop system asymptotically stable under continuous, state-feedback implementation. This assumption is essentially a stabilizability requirement for the system of eq 1. Using converse Lyapunov theorems,  $^{25-27}$  this assumption implies that there exist functions  $\alpha_i(\cdot)$ , i = 1, 2, 3, 4 of class  $\mathcal{K}$  and a continuous differentiable Lyapunov function V(x) for the closed-loop system that satisfy the following inequalities:

$$\alpha_{1}(|\mathbf{x}|) \le V(\mathbf{x}) \le \alpha_{2}(|\mathbf{x}|) \tag{3}$$

$$\frac{\partial V(x)}{\partial x}f(x, h_1(x), h_2(x), 0) \le -\alpha_3(|x|)$$
(4)

$$\left|\frac{\partial V(x)}{\partial x}\right| \le \alpha_4(|x|) \tag{5}$$

$$h_1(x) \in U_1, \qquad h_2(x) \in U_2 \tag{6}$$

for all  $x \in D \subseteq \mathbb{R}^n$  where *D* is an open neighborhood of the origin. We denote the region  $\Omega_{\rho} \subseteq D$  as the stability region of the closed-loop system under the controller  $(u_1, u_2) = h(x)$ . Note that explicit stabilizing control laws that provide explicitly defined stability regions  $\Omega_{\rho}$  for the closed-loop system have

been developed using Lyapunov techniques for nonlinear systems (see refs 28–30).

By continuity and the local Lipschitz property assumed for the vector field f and taking into account that both sets of the manipulated inputs  $u_1$  and  $u_2$  and the disturbance w are bounded, there exists a positive constant M such that

$$|f(x, u_1, u_2, w)| \le M$$
<sup>(7)</sup>

for all  $x \in \Omega_{\rho}$ ,  $u_1 \in U_1$ ,  $u_2 \in U_2$ , and  $w \in W$ . Furthermore, from the continuous differentiable property of the Lyapunov function V and the Lipschitz property of the vector field f, there exist positive constants  $L_{x}$ ,  $L_{w}$ ,  $L'_{x}$  and  $L'_{w}$  such that

$$\left| f(x, u_1, u_2, w) - f(x', u_1, u_2, 0) \right| \le L_x |x - x'| + L_w |w|$$

$$\left| \frac{\partial V}{\partial x} f(x, u_1, u_2, w) - \frac{\partial V}{\partial x} f(x', u_1, u_2, 0) \right|$$
(8)

$$\leq L'_{x}|x - x'| + L'_{w}|w| \tag{9}$$

for all  $x, x' \in \Omega_{\rho}, u_1 \in U_1, u_2 \in U_2$ , and  $w \in W$ 

In this work, we design a two-layer framework where the upper layer can transmit information to the lower layer and to the system control actuators. The lower layer can receive information from the upper layer and is able to transmit information to the control actuators. The following assumption is required to ensure stability of the process with this type of communication and defines how we group the full set of manipulated inputs into two groups  $u_1$  and  $u_2$ .

Assumption 1. We assume that for any fixed  $u_{1,E} \in U_{1}$ , there exists  $u_{2} \in U_{2}$  such that the following holds

$$\frac{\partial V(x)}{\partial x}f(x, u_{1,E}, u_2, 0) \le \frac{\partial V(x)}{\partial x}f(x, h_1(x), h_2(x), 0)$$
(10)

for all  $x \in \Omega_{\rho}$ .

**Remark 1.** Although there are currently no general methods for constructing Lyapunov functions for general nonlinear systems, quadratic Lyapunov functions (i.e.,  $V(x) = x^{T}Vx$ ) are typically used within the context of chemical process control applications and have been demonstrated to yield good estimates of closed-loop stability regions; please see also the Application to a Chemical Process Example section.

Remark 2. We note the stability region  $\Omega_{\rho}$  can be estimated for a given system and controller h(x) by the following procedure:  $\dot{V}(x)$ is evaluated for different values of x while the Lyapunov-based controller h(x) is applied to the nominal system of eq 1 with  $w(t) \equiv 0$ . Then,  $\Omega_{\rho}$  can be estimated as the level set of the Lyapunov function V(x) (ideally, the largest level set) where  $\dot{V}(x) \leq 0$ .

**Lyapunov-Based MPC.** To address stability of the closedloop system with model predictive control (MPC) and feasibility of the optimization problem, researchers<sup>25,31,32</sup> have combined the stability and robustness properties of the Lyapunov-based controller with the optimal control properties of model predictive control (MPC). The resulting MPC is the Lyapunov-based MPC (LMPC) and is characterized by the following optimization problem:

$$\min_{\substack{(u_1,u_2)\in S(\Delta)}} \int_{t_k}^{t_{k+N}} (|\tilde{x}(\tau) - x_s|_{Q_c} + |u_1(\tau) - u_{1,s}|_{R_{c,1}} + |u_2(\tau) - u_{2,s}|_{R_{c,2}}) d\tau$$
(11a)

s.t. 
$$\dot{\tilde{x}}(t) = f(\tilde{x}(t), u_1(t), u_2(t), 0)$$
 (11b)

$$\tilde{x}(t_k) = x(t_k) \tag{11c}$$

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$$u_1(t) \in U_1, \qquad \forall \ t \in [t_k, \ t_{k+N})$$
(11d)

$$u_2(t) \in U_2, \qquad \forall \ t \in [t_k, \ t_{k+N})$$
 (11e)

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$$\frac{\partial V}{\partial x} f(x(t_k), u_1(t_k), u_2(t_k), 0)$$

$$\leq \frac{\partial V}{\partial x} f(x(t_k), h_1(x(t_k)), h_2(x(t_k)), 0)$$
(11f)

where  $\tilde{x}$  is the predicted state evolution over the prediction horizon with the computed control input by the LMPC,  $S(\Delta)$ is the set of piecewise constant functions with period  $\Delta$ , N is the finite prediction horizon, and  $Q_c$ ,  $R_{c,1}$ , and  $\overline{R}_{c,2}$  are positive definite weighting matrices. In the optimization problem of eq 11, eq 11b is the nominal system of eq 1 used to predict the future evolution of the system; eq 11c is the initial condition of the optimization problem; eqs 11d and 11e define the control energy available to all manipulated inputs; eq 11f ensures that over the sampling period  $t \in [t_k, t_k + \Delta)$  the LMPC computes manipulated inputs that decrease the Lyapunov function by at least the rate achieved by the Lyapunov-based controller h(x) when implemented in a sample-and-hold fashion. The optimal solution of the optimization problem of eq 12 is denoted by  $u_1^*(t|t_k)$  and  $u_2^*(t|t_k)$  and is defined for  $t\in [t_k, t_{k+N}).$ 

Since for any initial condition  $x(t_0) \in \Omega_{\rho}$  the closed-loop system state is guaranteed to converge to a small neighborhood of the origin and the optimization problem of eq 11 is guaranteed to be feasible for any initial condition  $x(t_0) \in \Omega_{\rho}$ , the LMPC is said to inherit the stability region of the Lyapunov-based controller  $\Omega_{\rho}$ .

**Lyapunov-Based Economic MPC.** If instead of the conventional quadratic cost function, a general cost function is used which accounts for system economic considerations and we reformulate the Lyapunov-based constraint of eq 11f to allow the system to operate in a time-varying fashion about the steady-state by taking advantage of the stability region  $\Omega_{\rho}$  of the Lyapunov-based controller. The result is the Lyapunov-based economic MPC (LEMPC),<sup>17</sup> and it is defined by the following optimization problem:

$$\max_{(u_{1,E},u_{2,E})\in S(\Delta)} \int_{t_k}^{t_{k+N_E}} L_E(\tilde{x}(\tau), u_{1,E}(\tau), u_{2,E}(\tau)) \, \mathrm{d}\tau$$
(12a)

s.t. 
$$\dot{\vec{x}}(t) = f(\tilde{x}(t), u_{1,E}(t), u_{2,E}(t), 0)$$
 (12b)

$$\tilde{x}(t_k) = x(t_k) \tag{12c}$$

$$u_{1,E}(t) \in U_1, \qquad \forall \ t \in [t_k, \ t_{k+N})$$
(12d)

$$u_{2,E}(t) \in U_2, \qquad \forall \ t \in [t_k, \ t_{k+N})$$
(12e)

$$V(\tilde{x}(t)) \le \rho_e \ \forall \ t \in [t_k, \ t_{k+N}), \text{ if } V(x(t_k)) < \rho_e$$
(12f)

$$\frac{\partial V}{\partial x} f(x(t_k), u_1(t_k), u_2(t_k), 0)$$

$$\leq \frac{\partial V}{\partial x} f(x(t_k), h_1(x(t_k)), h_2(x(t_k)), 0),$$
if  $V(x(t_k)) \ge \rho_c$ 
(12e)

where the parameter  $\rho_e$  is used to denote a subset of  $\Omega_{\rho}$  where the system is allowed to evolve in a time-varying fashion. In the



Figure 1. Block diagram of the proposed two-layer integrated framework for dynamic economic optimization and process control with economic MPC in the upper layer and MPC in the lower layer. Both the upper and lower layers compute control actions that are applied to the process.

optimization problem of eq 12, the cost function of eq 12a is constructed to account directly for the economic measure of the process. The constraint of eq 12f is imposed when the current state  $x(t_k)$  of the system is inside the set  $\Omega_{\rho_e}$  and restricts the future predicted state evolution to remain in the region  $\Omega_{\rho_e}$ . This constraint defines mode 1 operation of LEMPC. The constraint of eq 12g is a similar Lyapunov-based constraint as eq 11f of the LMPC and is imposed when the current state  $x(t_k)$ is outside the set  $\Omega_{\rho_e}$  to drive the system into  $\Omega_{\rho_e}$ . This constraint defines mode 2 operation of the LEMPC. Refer to ref 17 for a detailed discussion and analysis of the LEMPC formulation of eq 12. The optimal solution of the optimization problem of eq 12 is denoted by  $u_{1,E}^*(t|t_k)$  and  $u_{2,E}^*(t|t_k)$  and is defined for  $t \in [t_k, t_{k+N_e})$ .

## PROPOSED TWO-LAYER ARCHITECTURE FOR DYNAMIC ECONOMIC OPTIMIZATION AND PROCESS CONTROL

In this section, we introduce the proposed two-layered dynamic economic optimization and control framework and provide a rigorous theoretical treatment of the stability properties of the closed-loop system of eq 1 with the proposed architecture.

**Dynamic Economic Optimization and Control Framework Formulation.** The proposed dynamic economic optimization and control framework consists of EMPC in the upper layer and MPC in the lower layer. A block diagram of the proposed framework is given in Figure 1. The upper layer EMPC is formulated as a LEMPC given by the optimization problem of eq 12. While LEMPC computes optimal input trajectories for both sets of manipulated inputs  $u_{1,E}^*$  and  $u_{2,E}^*$ , it sends control actions for the manipulated inputs  $u_1$  to the control actuators to be applied in a sample-and-hold fashion. It uses the full set of input trajectories  $u_{1,E}^*$  and  $u_{2,E}^*$  to compute the optimal operating trajectory over a finite operating window  $t_f$  which we explicitly define in the following definition.

**Definition 1.** The economically optimal state trajectory  $x_E^*(t)$  of the system of eq 1 over an operating window  $t_f$  is obtained by recursively solving

$$\dot{x}_{E}^{*}(t) = f(x_{E}^{*}(t), u_{1,E}^{*}(t), u_{2,E}^{*}(t), 0), \qquad t \in [t_{k}, t_{k+1}]$$
(13)

where  $t_k = t_0 + k\Delta_{E'} k = 0, 1, ..., and x_E(t_0) = x(t_0)$  for all  $t \in [t_k, t_k + t_f]$ .

The purpose of the lower layer is to force the system to track the optimal state trajectory  $x_E^*$ . The lower layer MPC is formulated as a LMPC. Since the optimal state trajectory is timevarying, we reformulate the cost function to track the economically optimal state trajectory  $x_E^*(t)$  and reformulate the Lyapunov-based constraint to allow for time-varying operation. Specifically, we add a constraint denoted as mode 1 operation to ensure the predicted system evolution remains bounded in  $\Omega_{\rho_c}$ . The resulting LMPC is given by the following optimization problem:

$$\min_{u_2 \in S(\Delta)} \int_{t_k}^{t_{k+N}} \left( |\tilde{x}(\tau) - x_E^*(\tau)|_{Q_c} + |u_2(\tau) - u_{2,E}^*(\tau)|_{R_c} \right) d\tau$$
(14a)

s.t. 
$$\dot{\tilde{x}}(t) = f(\tilde{x}(t), u_{1,E}^{*}(t), u_{2}(t), 0)$$
 (14b)

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

$$u_2(t) \in U_2, \qquad \forall \ t \in [t_k, \ t_{k+N}) \tag{14d}$$

$$\frac{\partial V}{\partial x} f(x(t_k), u_{1,E}^*(t_k), u_2(t_k), 0)$$

$$\leq \frac{\partial V}{\partial x} f(x(t_k), h_1(x(t_k)), h_2(x(t_k)), 0),$$
if  $V(x(t_k)) \ge \rho_e$ 
(14e)

$$V(x(t)) \le \rho_e \qquad \forall \ t \in [t_k, \ t_{k+N}), \qquad \text{if } V(x(t_k)) < \rho_e \tag{14f}$$

where the optimal solution is denoted as  $u_2^*(t)$  and defined for  $t \in [t_k, t_{k+N})$ . We note the two key differences between the LMPC of eq 11 and the LMPC of eq 14 are the added constraint of eq 14e which ensures the predicted evolution of the system is maintained in the region  $\Omega_{\rho_e}$  (the same  $\rho_e$  used in the upper layer LEMPC) and the quadratic cost function of eq 14a is formulated based on the optimal time-varying trajectory and not a steady-state point.

Remark 3. For simplicity, we have assumed that the sampling periods of the EMPC and MPC are the same. However, this two layer framework can easily be extended to the case where the sampling periods are not equal. In contrast, the prediction horizons of the two controllers are not assumed to be the same. In general, EMPC requires a much greater prediction horizon compared to MPC to ensure good closed-loop performance of the system.

**Implementation Strategy.** At the beginning of each operating window denoted  $t_0$ , the LEMPC operates in either

mode 1 if  $x(t_0) \in \Omega_{\rho_e}$  or mode 2 if  $x(t_0) \notin \Omega_{\rho_e}$  to solve the optimization problem given by eq 12. With the optimal solution  $u_1^*(t t t_k)$  and  $u_2^*(t t_k)$  defined for  $t \in [t_0, t_0 + t_f)$ , the economically optimal state trajectory is computed and the optimal trajectories are sent down to the lower layer LMPC. If the state  $x(t_0) \notin \Omega_{\rho,i}$  the LEMPC works in mode 2 and recomputes new optimal trajectories while employing a shrinking horizon strategy at every sampling period until the state converges to the set  $\Omega_{\rho,i}$ . Once the state converges to the set  $\Omega_{\rho,i}$  the LEMPC operates in mode 1 to compute the optimal trajectory over the remainder of the operating window. The implementation strategy of the LEMPC can be summarized as follows:

- 1. At time  $t_0$ , the LEMPC receives the system state  $x(t_0)$ and  $t_k := t_0$ . If  $x(t_0) \in \Omega_o$ , go to step 2; else, go to step 3.
- 2. The LEMPC operates in mode 1 to compute control actions that optimize the economic cost function; go to step 4.
- The LEMPC operates in mode 2 to compute control actions that drive the system into Ω<sub>ρ</sub>; go to step 4.
- The LEMPC computes the economically optimal state trajectory x<sup>\*</sup><sub>E</sub>(t) and input trajectories u<sup>\*</sup><sub>1,E</sub>(t) and u<sup>\*</sup><sub>2,E</sub>(t) for t ∈ [t<sub>k</sub>, t<sub>0</sub> + t<sub>f</sub>] and sends the optimal trajectories to the LMPC; go to step 5.
- 5. The LEMPC sends the control action  $u_{1,E}^*(t_k)$  to the control actuators to be applied in a sample-and-hold fashion for  $t \in [t_k, t_{k+1})$ ; go to step 5.1.
  - 5.1.  $k \leftarrow k + 1$ ; go to step 5.2.
  - 5.2. If  $t_k < t_0 + t_{fr}$  go to step 5.3; else, go to step 6.
  - 5.3. If LEMPC is operating in mode 2, go to step 5.3.1; else, go to step 5.
- 5.3.1. Decrease the prediction horizon of the LEMPC, i.e., N<sub>E,k</sub> = N<sub>E</sub> − k; go to step 5.3.2.
  5.3.2. If x(t<sub>k</sub>) ∈ Ω<sub>ρ</sub>, go to step 2; else, go to step 3.
  6. t<sub>0</sub> ← t<sub>0</sub> + t<sub>f</sub>; go to step 1.

At each sampling period denoted as  $t_k$ , the LMPC computes optimal control actions  $u_2^*(t)$  defined for  $t \in [t_k, t_{k+N})$ . It sends the optimal control action to be implemented in a sampleand-hold fashion over the sampling period  $t \in [t_k, t_{k+1})$ . The implementation strategy of the LMPC can be summarized as follows:

- 1. At time  $t_{k}$  the LMPC receives the system state  $x(t_k)$  and the optimal trajectories  $x_E^*(t)$ ,  $u_{1,E}^*(t)$ , and  $u_{2,E}^*(t)$  computed by the LEMPC. If  $x(t_k) \in \Omega_{\rho,\ell}$  go to step 2; else, go to step 3.
- 2. The LMPC operates in mode 1 to compute control actions that track the economically optimal state trajectory  $x_E^*(t)$ ; go to step 4.
- 3. The LMPC operates in mode 2 to compute control actions that drive the system into  $\Omega_{\alpha j}$  go to step 4.
- 4. Compute the optimal control action  $u_2^{re}(t)$  for  $t \in [t_{k}, t_{k+N})$ ; go to step 5.
- 5. The LMPC sends the control action  $u_2^*(t)$  to the control actuators to be applied in a sample-and-hold fashion for  $t \in [t_k, t_{k+1})$ ; go to step 6.
- 6.  $k \leftarrow k + 1$ ; go to step 1.

With this implementation strategy, we note several computational advantages over one-layer EMPC structures: when the LEMPC is operating in mode 1, the LEMPC problem is only computed once for each operating window. Also, the LMPC is less computationally complex than the LEMPC because the LMPC does not compute control actions for all of the manipulated inputs, and it also can use a smaller prediction horizon than the LEMPC. Furthermore, some inputs go to their maximum value and then switch to their minimum value after some time (like the reactant feed concentration in the CSTR second-order reaction example in ref 17). These inputs typically do not act on the system fast enough to drive the system back to its optimal state trajectories anyway so there really is not a need to recompute these trajectories (see the Application to a Chemical Process Example section).

**Stability Analysis.** In this section, we provide sufficient conditions whereby the closed-loop system with the proposed two-layer dynamic economic optimization and control framework is stable in the sense that the system state remains bounded in a compact set for all times. The first proposition provides an upper bound on the deviation of the state trajectory obtained using the nominal model (eq 1 with  $w(t) \equiv 0$ ) from the actual system state trajectory when the same control input trajectories are applied.

Proposition 1 (c.f. ref 32). Consider the systems

$$\dot{x}_{a}(t) = f(x_{a}(t), u_{1}(t), u_{2}(t), w(t))$$
  
$$\dot{x}_{b}(t) = f(x_{b}(t), u_{1}(t), u_{2}(t), 0)$$
(15)

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

$$|x_a(t) - x_b(t)| \le \alpha_w(t - t_0) \tag{16}$$

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

$$\alpha_w(\tau) = \frac{L_w \theta}{L_x} (e^{L_x \tau} - 1)$$
(17)

The following proposition bounds the difference between the Lyapunov function of two different states in  $\Omega_{\rho}$ .

**Proposition 2 (c.f. ref 32).** Consider the Lyapunov function  $V(\cdot)$  of the system of eq 1. There exists a quadratic function  $\alpha_V(\cdot)$  such that:

$$V(x) \le V(\hat{x}) + \alpha_V(|x - \hat{x}|) \tag{18}$$

for all  $x, \hat{x} \in \Omega_{\rho}$  with  $\alpha_V(s) = \alpha_4(\alpha_1^{-1}(\rho))s + M_V s^2$  where  $M_V$  is a positive constant.

Theorem 1 provides sufficient conditions such that the two layer dynamic economic optimization optimization and control framework guarantees that the state of the closed-loop system is always bounded in  $\Omega_{o}$ .

**Theorem 1.** Consider the system of eq 1 in a closed loop under the proposed two-layer framework with the LEMPC of eq 12 in the upper layer and the LMPC of eq 14 in the lower layer both based on the Lyapunov-based controller h(x) that satisfies the Lyapunov function conditions of eqs 3–5 and the input bound of eq 6. Let  $\varepsilon_w > 0$ ,  $\Delta > 0$ , and  $\rho > \rho_e > 0$  satisfy

$$\rho_e \le \rho - \alpha_V(\alpha_w(\Delta)) \tag{19}$$

and

$$-\alpha_3(\alpha_2^{-1}(\rho_e)) + L'_x M \Delta + L'_w \theta \le \frac{-\varepsilon_w}{\Delta}$$
(20)

If  $x(t_0) \in \Omega_{\rho}$ ,  $N \ge 1$ , and  $N_E \ge 1$ , then the state x(t) of the closed-loop system is always bounded in  $\Omega_{\rho}$ .

*Proof.* The proof consists of two parts. We first prove that the optimization problems of eqs 12 and 14 are feasible for all

states  $x \in \Omega_{\rho}$ . Subsequently, we prove that the closed-loop state of the system is always bounded in  $\Omega_{\rho}$ .

*Part 1.* When x(t) is maintained in  $\Omega_{\rho}$  (which will be proved in Part 2), both the LEMPC of eq 12 and LMPC of eq 14 optimization problems are feasible. The feasibility of the LEMPC follows because the input trajectory u(t), such that  $(u_1(t), u_2(t)) = h(x(t_{k+q})), \forall t \in [t_{k+q}, t_{k+q+1})$  with q = 0, ..., $N_E - 1$  is a feasible solution to the optimization problem since such trajectory satisfies the input constraints and the Lyapunovbased constraints for both mode 1 and mode 2 operation. This is guaranteed by the closed-loop stability property of the Lyapunov-based controller h(x). The feasibility of the LMPC follows because there exists an input trajectory  $u_1(t)$  that decreases the Lyapunov function by at least the rate given by the Lyapunov-based controller as a consequence of Assumption 1.

*Part 2.* We prove that for any system state starting within the set  $\Omega_{\rho}$  that the system state will stay inside of  $\Omega_{\rho}$  for all time (i.e.,  $\Omega_{\rho}$  is an invariant set). To accomplish this, we must consider two cases. First, we assume that the system state  $x(t_k) \in \Omega_{\rho_c}$  and show that  $x(t_{k+1}) \in \Omega_{\rho}$ . Second, we show that if  $x(t_k) \in \Omega_{\rho} \setminus \Omega_{\rho,j}$  then the system state remains in the set  $\Omega_{\rho}$  and after a finite amount of sampling periods converges to the set  $\Omega_{\rho,c}$ .

When  $x(t_k) \in \Omega_{\rho,i}$  from the constraint of eq 14e, we obtain that  $\tilde{x} \in \Omega_{\rho,i}$ . By Propositions 1 and 2, we have that

$$V(x(t_{k+1})) \le V(\tilde{x}(t_{k+1})) + \alpha_V(\alpha_w(\Delta))$$
(21)

Since  $V(\tilde{x}(t_{k+1})) \leq \rho_{e^{t}}$  if the condition of eq 19 is satisfied, we can conclude that

 $x(t_{k+1}) \in \Omega_{\rho}$ 

When  $x(t_k) \in \Omega_{\rho} \setminus \Omega_{\rho,j}$  from the constraint of eq 14e and the condition of eq 4, we can write

$$\frac{\partial V(x(t_k))}{\partial x} f(x(t_k), u_{1,E}^*, u_2^*(t_k), 0) \\
\leq \frac{\partial V(x(t_k))}{\partial x} f(x(t_k), h_1(x(t_k)), h_2(x(t_k)), 0) \\
\leq -\alpha_3(|x(t_k)|)$$
(22)

The time derivative of the Lyapunov function along the computed optimal trajectories  $u_{1,E}^*$  and  $u_2^*$  for  $\tau \in [t_k, t_{k+1})$  can be written as follows

$$\dot{V}(x(\tau)) = \frac{\partial V(x(\tau))}{\partial x} f(x(\tau), u_{1,E}^*(t_k), u_2^*(t_k), w(\tau))$$
(23)

Adding and subtracting the term  $\{\partial V[x(t_k)]/\partial x\}f(x(t_k), u_{1,E}^*(t_k), u_2^*(t_k), 0)$  to/from the above equation and considering eq 22, we have

$$\dot{V}(x(\tau)) \leq -\alpha_{3}(|x(t_{k})|) + \frac{\partial V(x(\tau))}{\partial x} \\ \times f(x(\tau), u_{1,E}^{*}(t_{k}), u_{2}^{*}(t_{k}), w(\tau)) \\ - \frac{\partial V(x(t_{k}))}{\partial x} f(x(t_{k}), u_{1,E}^{*}(t_{k}), u_{2}^{*}(t_{k}), 0)$$
(24)

Due to the fact that the disturbance is bounded  $|w| \le \theta$  and the Lipschitz properties of eq 9, we can write

$$\dot{V}(x(\tau)) \le -\alpha_3(|x(t_k)|) + L'_x|x(\tau) - x(t_k)| + L'_w\theta$$
(25)

Taking into account eq 7 and the continuity of x(t), the following bound can be written for all  $\tau \in [t_k, t_{k+1})$ 

$$|x(\tau) - x(t_k)| \le M\Delta \tag{26}$$

Substituting eq 26 into eq 25 and noting  $x(t_k) \in \Omega_{\rho} \setminus \Omega_{\rho, \rho}$  the inequality of eq 25 becomes

$$\dot{V}(x(\tau)) \le -\alpha_3(\alpha_2^{-1}(\rho_e)) + L'_x M \Delta + L'_w \theta$$
<sup>(27)</sup>

If the condition of eq 20 is satisfied, then there exists  $\varepsilon_w > 0$ such that the following inequality holds for  $x(t_k) \in \Omega_{\rho} \backslash \Omega_{\rho_e}$ 

 $\dot{V}(x(t)) \leq -\varepsilon_w/\Delta, \qquad \forall \ t = [t_k, \ t_{k+1})$ 

Integrating this bound on  $t \in [t_k, t_{k+1})$ , we obtain that

$$V(x(t_{k+1})) \le V(x(t_k)) - \varepsilon_w \tag{28}$$

$$V(x(t)) \le V(x(t_k)), \qquad \forall \ t \in [t_k, \ t_{k+1})$$
(29)

for all  $x(t_k) \in \Omega_{\rho} \setminus \Omega_{\rho_c}$ . Using eq 29 recursively, it is proved that, if  $x(t_k) \in \Omega_{\rho} \setminus \Omega_{\rho_c}$  the state converges to  $\Omega_{\rho_c}$  in a finite number of sampling times without leaving the stability region  $\Omega_{\rho}$ .

**Remark 4.** We note if the sampling periods of the upper and lower layers are different, one could take  $\Delta = \max{\{\Delta_1, \Delta_2\}}$  where  $\Delta_1$  and  $\Delta_2$  are the sampling periods of the upper and lower layer, respectively.

#### APPLICATION TO A CHEMICAL PROCESS

We implement the proposed two-layer architecture for dynamic economic optimization and process control on a benchmark chemical reactor example previously studied in the context of forced periodic operation.<sup>9,16</sup> Consider a nonisothermal CSTR with a coolant jacket to remove heat from the reactor where ethylene oxide (C<sub>2</sub>H<sub>4</sub>O) is produced from the catalytic oxidation of ethylene with air. Two combustion reactions occur that consume both the ethylene and ethylene oxide. The reactions are given by

$$C_2H_4 + \frac{1}{2}O_2 \xrightarrow{r_1} C_2H_4O$$
(30)

$$C_2H_4 + 3O_2 \xrightarrow{r_2} 2CO_2 + 2H_2O$$
(31)

$$C_2H_4O + \frac{5}{2}O_2 \xrightarrow{r_3} 2CO_2 + 2H_2O$$
 (32)

where  $r_{ii}$  i = 1, 2, 3 is the reaction rate of the *i*th reaction and the reaction rate expressions are

$$r_1 = k_1 \exp\left(\frac{-E_1}{RT}\right) P_E^{0.5}$$
(33)

$$r_2 = k_2 \exp\left(\frac{-E_2}{RT}\right) P_E^{0.25}$$
(34)

$$r_3 = k_3 \exp\left(\frac{-E_3}{RT}\right) P_{\rm EO}^{0.5} \tag{35}$$

where  $k_i$  and  $E_i$ , i = 1, 2, 3 are the reaction rate constant and activation energy, respectively, for the *i*th reaction, *T* is the temperature, *R* is the gas constant, and  $P_j$  is the partial pressure of the *j*th component in the reactor where j = E, EO denotes ethylene and ethylene oxide, respectively. These results are from ref 33 where Alfani and Carberry studied catalytic oxidation of ethylene using an unmodified, commercial catalyst and are based on data from the temperature range 523-573 K. Ideal gas is assumed, and the concentrations of the j = E, EO component can be written

$$C_j = \frac{P_j}{RT} \tag{36}$$

where  $C_j$  is the concentration of the *j*th component in the reactor. The states of the system are

$$\begin{aligned} x_1 &= \rho / \rho_{\rm ref}, \quad x_2 &= C_E / C_{\rm ref}, \quad x_3 &= C_{\rm EO} / C_{\rm ref}, \\ x_4 &= T / T_{\rm ref} \end{aligned}$$

where  $\rho/\rho_{\rm ref}$  is the normalized vapor density in the reactor,  $C_{\rm E}/C_{\rm ref}$  is the normalized ethylene concentration in the reactor,  $C_{\rm EO}/C_{\rm ref}$  is the normalized ethylene oxide concentration in the reactor, and  $T/T_{\rm ref}$  is the normalized reactor temperature. The manipulated inputs are

$$u_1 = Q_f / Q_{ref}, \quad u_2 = C_{E,f} / C_{ref}, \quad u_3 = T_c / T_{ref}$$

where  $Q_{\rm f}/Q_{\rm ref}$  is the normalized volumetric flow rate of the reactor feed,  $C_{\rm E,f}/C_{\rm ref}$  is the normalized ethylene concentration of the reactor feed, and  $T_{\rm c}/T_{\rm ref}$  is the normalized coolant temperature. The model describing the dynamic behavior of the reactor obtained through first principles under standard modeling assumptions (i.e., ideal gas, constant heat capacity, etc.) is

$$\frac{dx_1}{dt} = u_1(1 - x_1 x_4) \tag{37}$$

$$\frac{\mathrm{d}x_2}{\mathrm{d}t} = u_1(u_2 - x_2x_4) - A_1 \mathrm{exp}(\gamma_1/x_4)(x_2x_4)^{1/2} - A_2 \mathrm{exp}(\gamma_2/x_4)(x_2x_4)^{1/4}$$
(38)

$$\frac{\mathrm{d}x_3}{\mathrm{d}t} = -u_1 x_3 x_4 + A_1 \exp(\gamma_1 / x_4) (x_2 x_4)^{1/2} - A_3 \exp(\gamma_3 / x_4) (x_3 x_4)^{1/2}$$
(39)

$$\frac{\mathrm{d}x_4}{\mathrm{d}t} = \frac{u_1}{x_1}(1-x_4) + \frac{B_1}{x_1} \exp(\gamma_1/x_4)(x_2x_4)^{1/2} \\
+ \frac{B_2}{x_1} \exp(\gamma_2/x_4)(x_2x_4)^{1/4} + \frac{B_3}{x_1} \exp(\gamma_3/x_4)(x_3x_4)^{1/2} \\
- \frac{B_4}{x_1}(x_4-u_3)$$
(40)

where the parameters are given in Table 1 and are taken from refs 9 and 16. We note that the parameters, states, inputs, and time have been normalized and are unitless. To integrate the

Table 1. Dimensionless Process Model Parameters of theEthylene Oxidation  $CSTR^a$ 

| parameter | value   | parameter      | value  |
|-----------|---------|----------------|--------|
| $A_1$     | 92.80   | $\gamma_1$     | -8.13  |
| $A_2$     | 12.66   | $\gamma_2$     | -7.12  |
| $A_3$     | 2412.71 | γ <sub>3</sub> | -11.07 |
| $B_1$     | 7.32    |                |        |
| $B_2$     | 10.39   |                |        |
| $B_3$     | 2170.57 |                |        |
| $B_4$     | 7.02    |                |        |

<sup>a</sup>The parameters are taken from ref 16.

ordinary differential equations (ODEs), the explicit Euler method is used with integration step size of 0.0001.

The CSTR system of eqs 37–40 has an asymptotically stable steady-state

$$x_{\rm s}^{\rm T} = [0.998, 0.424, 0.032, 1.002]$$
 (41)

which corresponds to the steady-state input

$$u_s^{-1} = \begin{bmatrix} 0.35, \ 0.5, \ 1.0 \end{bmatrix} \tag{42}$$

The maximum available control energy is considered bounded in the following set:  $u_1 \in [0.0704, 0.7042]$ ,  $u_2 \in [0.2465, 2.4648]$ , and  $u_3 \in [0.6, 1.1]$ . The control objective is to optimize the time-averaged yield of ethylene oxide by operating the CSTR in a time-varying fashion around the stable steadystate (mode 1 operation only). The time-averaged yield of ethylene oxide over an operating window  $t_f$  is given by

$$Y(t_{\rm f}) = \frac{\int_0^{t_{\rm f}} u_1(\tau) x_4(\tau) x_3(\tau) \, \mathrm{d}\tau}{\int_0^{t_{\rm f}} u_1(\tau) u_2(\tau) \, \mathrm{d}\tau}$$
(43)

which is a measure of the amount of ethylene oxide leaving the CSTR compared to the amount of ethylene fed into the CSTR. To provide a fair comparison between the closed-loop performance with the proposed two-layer framework and the closed-loop performance when feeding the reactant material uniformly to the reactor, we impose an additional constraint on the EMPC to limit the average amount of ethylene fed into the process over the operating window to be the same as uniformly distributing the reactant material to the CSTR. The constraint is given by

$$\frac{1}{t_{\rm f}} \int_0^{t_{\rm f}} u_1(\tau) u_2(\tau) \, \mathrm{d}\tau = u_{s_1 1} u_{s_2 2} = 0.175 \tag{44}$$

where  $u_{s,1}$  and  $u_{s,2}$  are the steady-state inlet volumetric flow rate and ethylene concentration, respectively. Since the average ethylene fed to the CSTR over the operating window  $t_{\rm f}$  is fixed, the economic cost that the EMPC attempts to maximizes is

$$\int_{0}^{t_{\rm f}} L(x(t), u(t)) = \int_{0}^{t_{\rm f}} u_1(\tau) x_4(t) x_3(t) \,\mathrm{d}\tau \tag{45}$$

which is equivalent to maximizing the time-averaged yield over the period  $t_{\rm f}$ .

In the implemented two-layer dynamic optimization and control framework, we partition the manipulated inputs into two sets as in eq 1. The first set of manipulated inputs consists of  $u_1$  and  $u_2$  for which the upper layer LEMPC of eq 12 computes control actions and applies them to the closed-loop system. The second set of manipulated inputs consists of the manipulated input  $u_3$  for which the LMPC of eq 14 computes control actions that are applied in a sample-and-hold fashion to the closed-loop system. The LEMPC also sends the optimal operating trajectory  $x_E^*(t)$  over one operating period to the lower LMPC layer to force the system to track this trajectory.

To characterize the closed-loop stability region  $\Omega_{\rho,r}$  we define the Lyapunov-based controller  $u_3 = h(x) = K(x_3 - x_{s,3}) + u_{s,3}$  as a proportional controller with K = 0.1 and use a quadratic Lyapunov function defined as  $V(x) = (x - x_s)^T P(x - x_s)$  with the positive definite matrix *P* defined as P = diag[10, 0.01, 10, 10]. With the given CSTR system, the Lyapunov-based controller, and Lyapunov function, we are able to estimate the closed-loop stability region as  $\rho_e = 0.2$ . This Lyapunov-based controller h(x)is used in the design of the upper layer LEMPC and the lower



**Figure 2.** Design of the open-loop periodic operation strategy over one period  $\tau$ .



Figure 3. Open-loop CSTR (a) state trajectories and (b) input trajectories with the periodic operating strategy shown in Figure 2.

layer LMPC. The prediction horizon of the LEMPC and LMPC are  $N_E = t_f/\Delta$  and N = 3, respectively. The weighting matrices of the LMPC are  $Q_c = P$ , and  $R_c = 0.01$  which have been tuned to achieve close tracking of the optimal trajectory. The optimization problems of eq 12 and 14 are solved using the open-source software Ipopt.<sup>34</sup>



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**Figure 4.** Closed-loop CSTR (a) state trajectories and (b) input trajectories with the proposed two-layer dynamic economic optimization and control framework.

In the simulations, we implement the proposed two-layer dynamic optimization and process control structure (upper layer LEMPC and lower layer LMPC) and compare the closedloop economic performance of the process under the proposed architecture with the economic performance of the forced periodic operating strategy proposed in ref 16. We also demonstrate the ability to handle process noise of the closedloop system with the proposed two-layer framework.

We first motivate the use of EMPC over steady-state operation and the time-varying operating strategy proposed in ref 16. Specifically, we implement a similar periodic control strategy as in ref 16 which varies the inlet feed flow rate and feed concentration in an open-loop periodic fashion as shown in Figure 2 while keeping the reactor coolant temperature fixed. The parameters we use for this control strategy are  $\tau = 46.8$ ,  $a_1 = 0.073$ ,  $a_2 = 0.500$ ,  $a_3 = 0.514$ ,  $a_4 = 0.941$ , and k = 0, 1, ... which are similar parameters to the ones calculated in ref 16. To compare this strategy to using EMPC, we implement the upper layer LEMPC only to compute control actions for the inlet feed flow rate and feed concentration in a closed-loop fashion for the system without uncertainties or process noise.



**Figure 5.** State-space evolution in the  $x_2-x_3$  phase plane of the CSTR system given by eqs 37–40 with the LEMPC of eq 12 operating in mode 1 only and with the periodic control strategy shown in Figure 2.

The LEMPC uses a prediction horizon of  $N_E = 468$  with a sampling period of  $\Delta = 0.1$  chosen to cover the entire operating window (i.e.,  $t_f = \tau = 46.8$ ). The LEMPC is implemented with a shrinking horizon at each sampling time where the prediction horizon is equal to  $N_{E,k} = N_E - k$  at each sampling period until the end of the operating window when the prediction horizon is reset to  $N_E$  and k = 0.

The CSTR system is initialized at

$$x_0^{-1} = [0.997, 1.264, 0.209, 1.004]$$
 (46)

which corresponds to an initial state on the stable limit cycle that the process with the periodic strategy follows. Simulations are carried out with the periodic control strategy and the LEMPC over 10 operating windows. The evolution of the CSTR for both cases is plotted in Figure 3 with the open-loop periodic operation and Figure 4 with the upper layer LEMPC. The state-space evolutions of the two strategies are plotted in the  $x_2 - x_3$  phase plane (Figure 5). From these figures, we observe the system with the two operating strategies approaches different limit cycles. For the case with LEMPC, the time-averaged yield over the entire time-interval of the process simulation is 9.97% compared to the 7.93% with the periodic operation. The latter agrees with the yield of 7.90% reported in ref 16, and the difference likely lies in the small differences in the model parameters used. We note that if we were to initialize the CSTR system with the same initial point and distribute the material uniformly over the operating window by setting the inlet volumetric flow rate and ethylene concentration to a fixed value at its steady-state value the average yield is 6.63%. If instead, we initialize the system at the steady-state and maintain the feed conditions constant, the average yield is 6.41%. Therefore, the CSTR operated with EMPC has a clear performance benefit as opposed to steadystate operation and the open-loop periodic operation strategy.

To increase the robustness of the closed-loop CSTR system and to deal with disturbances, uncertainties, and modeling error while decreasing the computational demand, we implement the proposed two-layer dynamic economic optimization and process control framework to the system. With this strategy,



**Figure 6.** Closed-loop CSTR (a) state trajectories and (b) input trajectories with the proposed two-layer dynamic economic optimization and control framework.

LEMPC, operating in mode 1 only, computes optimal state and input trajectories at the beginning of each operating window. The LEMPC sends down the trajectories to the LMPC and the LMPC works to force the system to track this operating policy. We first implement the proposed two-layer framework to the system without process noise and initialize the system at the same initial condition as in the previous simulations. The closed-loop evolution of the CSTR is plotted in Figure 6. As we can see in the figure, the LMPC is able to force the system to track the optimal state trajectory. This is expected because the sampling periods of the upper and lower layer are the same and the closed-loop system is subjected to no uncertainities or disturbances.

We note that the computation time of the lower layer LMPC is insignificant compared to the computation time of the upper layer LEMPC. Our proposed two-layer framework only solves the LEMPC optimization problem once every operating window. At the beginning of the operating window, the computational burden of our two-layer framework compared to the one-layer LEMPC would be the only time the two approaches would be comparable (theoretically, the computational time of the two approaches would be the same). For all other times, the



Figure 7. Closed-loop CSTR (a) state trajectories and (b) input trajectories with the proposed two-layer dynamic economic optimization and control framework and with process noise added to the system states.

computation of the LMPC which computes control actions for the set of manipulated inputs  $u_2$  is insignificant compared to the one-layer LEMPC. The one-layer LEMPC would have a larger prediction horizon in general and would need to compute control actions for both sets of manipulated inputs:  $u_1$  and  $u_2$ .

Finally, we add significant process noise to the system states. The noise is assumed to be bounded Gaussian white noise with zero mean and standard deviation of  $\sigma_w = [0.005, 0.03, 0.01,$ 0.02] and bounds given by  $\theta = [0.02, 0.1, 0.03, 0.08]$ . To simulate the process noise, a new random number is generated and applied to the process over each sampling period. The results of a closed-loop simulation are plotted in Figure 7. Because of the added process noise, the lower layer LMPC is not able to force the closed-loop system to fully track the economically optimal state trajectory. Also, the added process noise has an effect on the closed-loop economic cost. Specifically, the time-averaged yield of the closed-loop system with the proposed two-layer framework is 10.3% with the added process disturbance and 10.4% without the added process disturbance. It is important to point out that even with the process noise added, the two-layer framework is able to outperform steadystate operation and the periodic operating strategy without process noise.

## CONCLUSIONS

In this work, we proposed a two-layer framework for dynamic economic optimization and process control that reduces the computational demand required for one-layer economic MPC schemes. In the upper layer, Lyapunov-based economic MPC (LEMPC) was used to compute optimal operating trajectories and control actions for some of the process manipulated inputs. The lower layer, utilizing Lyapunov-based MPC (LMPC), is used to force the system to track the optimal operating policy computed by the upper layer. We proved boundedness of the closed-loop system state with the proposed framework. Lastly, we demonstrated through a chemical process example that the proposed framework achieves stability and yields improved closed-loop economic performance compared to steady-state operation.

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#### Notes

The authors declare no competing financial interest.

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