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Integrating dynamic economic optimization and model predictive control for optimal operation of nonlinear process systems

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ABSTRACT

In this work, we propose a conceptual framework for integrating dynamic economic optimization and model predictive control (MPC) for optimal operation of nonlinear process systems. First, we introduce the proposed two-layer integrated framework. The upper layer, consisting of an economic MPC (EMPC) system that receives state feedback and time-dependent economic information, computes economically optimal time-varying operating trajectories for the process by optimizing a time-dependent economic cost function over a finite prediction horizon subject to a nonlinear dynamic process model. The lower feedback control layer may utilize conventional MPC schemes or even classical control to compute feedback control actions that force the process state to track the time-varying operating trajectories computed by the upper layer EMPC. Such a framework takes advantage of the EMPC ability to compute optimal process time-varying operating policies using a dynamic process model instead of a steady-state model, and the incorporation of suitable constraints on the EMPC allows calculating operating process state trajectories that can be tracked by the control layer. Second, we prove practical closed-loop stability including an explicit characterization of the closed-loop stability region. Finally, we demonstrate through extensive simulations using a chemical process model that the proposed framework can both (1) achieve stability and (2) lead to improved economic closed-loop performance compared to real-time optimization (RTO) systems using steady-state models.

1. Introduction

Economic optimization of chemical processes has traditionally been addressed through a two-layered architecture. In the upper layer, real-time optimization (RTO) carries out economic process optimization by computing optimal process operation set-points using steady-state process models. These set-points are used by the feedback control systems in the lower layer, typically designed via model predictive control (MPC) methods, to force the process to operate on these steady-states (Backx, Bosgra, & Marquardt, 2000; Marlin & Hrymak, 1997). MPC has been widely adopted in the chemical process industry because of its ability to optimally control multiple-input multiple-output nonlinear systems by solving an on-line optimization problem subject to input and state constraints (García, Prett, & Morari, 1989; Mayne, Rawlings, Rao, & Scokaert, 2000) and minimizes a typically quadratic performance index along a finite prediction horizon. The main disadvantage of this traditional two-layer approach to economic process optimization with RTO and MPC is that RTO does not account for process dynamics or guarantee that the computed set-points are reachable (Rawlings, Bonné, Jørgensen, Venkat, & Jørgensen, 2008). In recent years, numerous calls for the development of the so-called "smart manufacturing paradigm" have led to several attempts to integrate MPC and economic optimization of chemical processes to deal with variable demand, changing energy prices, variable feedstock, and product transitions (Adetola & Guay, 2010; Backx et al., 2000; Tvrzská de Gouvêa & Odloak, 1998; Engell, 2007; Kadam & Marquardt, 2007; Rawlings & Amrit, 2009; Zanin, Tvrzská de Gouvêa, & Odloak, 2002).

Early attempts on integrating MPC and economic optimization have primarily focused on two strategies: (1) integrating steady-state optimization directly in the MPC as in Tvrzská de Gouvêa and Odloak (1998), Zanin et al. (2002), and Yousfi and Tournier (1991) and (2) a two-layer approach similar to traditional control architectures with RTO and MPC that incorporates a dynamic process model in place of a steady-state model in the upper layer called dynamic real-time optimization (D-RTO) (Kadam & Marquardt, 2007; Kadam et al., 2003; Würth, Hannemann, & Marquardt, 2009, 2011; Würth, Rawlings, & Marquardt, 2009; Zhu, Hong, & Wang, 2004). In recent work, the MPC has been

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extended to solve optimization problems with general economic cost functions replacing the convectional quadratic cost of the standard MPC. This combines dynamic economic process optimization and feedback control into one layer. Several economic MPC (EMPC) schemes have been proposed (see Amrit, Rawlings, & Angeli, 2011; Chen, Heidarinejad, Liu, & Christofides, 2012; Diehl, Amrit, & Rawlings, 2011; Heidarinejad, Liu, & Christofides, 2012a, 2012b; Hovgaard, Larsen, Edlund, & Jørgensen, 2012; Huang, Harinath, & Biegler, 2011; Ma, Qin, Salsbury, & Xu, 2012; Rawlings & Amrit, 2009 and the references therein). In Heidarinejad et al. (2012a), general methods were proposed to design an EMPC using Lyapunov-based techniques capable of optimizing closed-loop performance with respect to general economic considerations for nonlinear systems. Moreover, this approach allows for an explicit characterization of the set of initial conditions whereby closed-loop stability and feasibility of the EMPC optimization problem are guaranteed.

While the proposed EMPC approaches have demonstrated closed-loop economic performance improvement, these approaches treat dynamic economic process optimization and control in a one layer approach. This shift from the traditional two layer control paradigm to a one layer framework requires a complete redesign of the existing control architectures. Additionally, considering that EMPC must use a sufficiently large prediction horizon to adequately account for a time-varying economic cost, the EMPC optimization problem may not be solved fast enough to control a process in real-time. While many D-RTO structures have been proposed throughout the literature (for example, Kadam & Marquardt, 2007; Würth et al., 2011; Zhu et al., 2004), many of the two-layered D-RTO and MPC systems proposed are characterized by a lack of rigorous theoretical treatment including the constraints required on the upper level dynamic economic optimization problem to guarantee that the computed optimal time-varying reference state trajectories can be tracked by the lower process control layer as well as an explicit characterization of the set of initial conditions whereby closed-loop stability and feasibility are guaranteed in the lower layer.

Accounting for these considerations, we design, in the present work, a two-layered dynamic economic optimization and control framework. In the upper layer, an EMPC is designed to compute economically optimal time-varying state trajectories in an on-line fashion using real-time measurements. In the lower layer, a LMPC system is used to force the system to track the economically optimal state trajectories taking advantage of its stability and robustness properties (see Christofides & El-Farra, 2005; Mhaskar, El-Farra, & Christofides, 2005, 2006; Muñoz de la Peña & Christofides, 2008). Lyapunov techniques are used to characterize, a priori, the set of initial conditions starting from where feasibility and closed-loop stability are guaranteed. Through rigorous theoretical treatment, we prove practical closed-loop stability of the proposed integrated dynamic economic optimization and control framework. We demonstrate through extensive simulations using a CSTR chemical process model with a time-dependent economic cost function that such an integrated control paradigm can both (1) render the closed-loop time-varying state evolution in a bounded region and (2) perform economically better than traditional RTO systems using steady-state models.

2. Preliminaries

2.1. 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., $|x|_Q = x^T Q x$). A continuous function $\alpha : [0,a) \to [0,\infty)$ belongs to class $\mathcal{K}$ if it is strictly increasing and satisfies $\alpha(0) = 0$. We use $\Omega_{\rho(x_E)}$ to denote the set $\Omega_{\rho(x_E)} := \{e \in \mathbf{R}^{n_x} \,|\, V(e,x_E) \le \rho(x_E)\}$ for a fixed $x_E \in \Gamma$. The symbol diag(v) denotes a square diagonal matrix with diagonal elements equal to the vector v and the symbol

$$\operatorname*{proj}_{\Gamma}(x)$$

denotes the projection of x onto the set Γ.

2.2. Class of process models

In this work, we consider the class of nonlinear systems described by the following state-space model:

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

where $x(t) \in \mathbf{R}^{n_x}$ is the state vector, $u(t) \in U \subset \mathbf{R}^{n_u}$ is the manipulated input vector, $w(t) \in \mathbf{R}^{n_w}$ is the disturbance vector. The inputs are restricted to be in a nonempty convex set defined as $U := \{u \in \mathbf{R}^{n_u} \,|\, |u_i| \le u_i^{\max},\ i = 1,\ldots,n_u\}$. We assume that f is locally Lipschitz on $\mathbf{R}^{n_x} \times \mathbf{R}^{n_u} \times \mathbf{R}^{n_w}$ and the disturbance vector is bounded

$$|w(t)| \le \theta \tag{2}$$

where $\theta > 0$.

We propose a dynamic economic optimization and control framework to force the system of Eq. (1) to track slowly time-varying operating policies. The slowly time-varying trajectory vector is denoted as $x_E(t) \in \Gamma \subset \mathbf{R}^{n_x}$, where Γ is a compact (closed and bounded) set and the rate of change of the reference trajectory is bounded by

$$|\dot{x}_E(t)| \le \gamma_E \tag{3}$$

We define the deviation between the actual state trajectory $x(t)$ and the slowly-varying reference trajectory $x_E(t)$ as

$$e(t) = x(t) - x_E(t) \tag{4}$$

with its dynamics described by

$$\begin{aligned} \dot{e}(t) &= f(x(t),u(t),w(t)) - \dot{x}_E(t) \\ &= f(e(t)+x_E(t),u(t),w(t)) - \dot{x}_E(t) \\ &:= g(e(t),x_E(t),\dot{x}_E(t),u(t),w(t)) \end{aligned} \tag{5}$$

We assume that the system of Eq. (5) has a continuously differentiable, isolated equilibrium for each fixed $x_E \in \Gamma$ (i.e., there exists a u_E for a fixed x_E to make $e = 0$ the equilibrium of Eq. (5))

$$g(0,x_E,0,u_E,0) = 0 \tag{6}$$

Remark 1. The assumption that the system of Eq. (1) has an equilibrium for every fixed $x_E \in \Gamma$ is a necessary assumption to guarantee that the reference trajectory can be tracked. While this assumption does require the system to have enough degrees of freedom (e.g., one manipulated input for each time-varying state to track), a system with many states most likely will not include all states in the economic cost. In this case, only a few states would be forced to track reference trajectories. If we remove this assumption and the system is driven away from perfectly tracking the slowly-varying trajectory $x_E(t)$, due to a disturbance for example, no guarantee can be made that the system will ever be driven back to the slowly-varying reference trajectory.

2.3. Stability assumption

We need to make certain assumptions about the system of Eq. (5) to guarantee that the slowly-varying state trajectory $x_E(t)$ can be tracked. For each fixed $x_E \in \Gamma$, we assume that there exists a Lyapunov-based controller $h(e(t),x_E)$ that makes the origin $e = 0$ of the nonlinear system given by Eq. (5) without uncertainty ($w(t) \equiv 0$) asymptotically stable under continuous implementation.

This assumption is essentially equivalent to the assumption that the nominal system of Eq. (1) is stabilizable at each $x_E \in \Gamma$ (i.e., Γ is an equilibrium manifold). Using converse theorems (Khalil, 2002; Lin, Sontag, & Wang, 1996; Massera, 1956; Mhaskar et al., 2005), this assumption implies that for each fixed $x_E \in \Gamma$ there exists class $\mathcal{K}$ functions $\alpha_i(\cdot)$, $i=1, 2, 3, 4, 5$ and a continuously differentiable Lyapunov function $V(e,x_E)$ satisfying

$$\alpha_1(|e|) \le V(e,x_E) \le \alpha_2(|e|), \tag{7}$$

$$\frac{\partial V}{\partial e} g(e,x_E,0,h(e,x_E),0) \le -\alpha_3(|e|), \tag{8}$$

$$\left|\frac{\partial V}{\partial e}\right| \le \alpha_4(|e|), \tag{9}$$

$$\left|\frac{\partial V}{\partial x_E}\right| \le \alpha_5(|e|), \tag{10}$$

$$h(e,x_E) \in U, \tag{11}$$

for all $e \in D_s \subseteq \mathbf{R}^{n_x}$, where D_s is an open neighborhood of the origin. While the Lyapunov function constraints of Eqs. (7)–(9) are similar to the constraints typically used for standard Lyapunov functions, the constraint of Eq. (10) is needed to account for the time-varying reference trajectory $x_E(t)$. We denote the region $\Omega_{\rho*}$ as the intersection of stability regions $\Omega_{\rho(x_E)}$ of the closed-loop system under the Lyapunov-based controller $h(e,x_E)$ for each fixed equilibrium $x_E \in \Gamma$. Note that explicit stabilizing control laws that provide explicitly defined stability regions $\Omega_{\rho(x_E)}$ for the closed-loop system have been developed using Lyapunov techniques for various classes of nonlinear systems (see Christofides & El-Farra, 2005; El-Farra & Christofides, 2003; Kokotović & Arcak, 2001; Lin & Sontag, 1990).

By continuity, the local Lipschitz property assumed for the vector field f and taking into account that the manipulated inputs u_i, $i=1, 2, \ldots, n_u$ are bounded in nonempty convex sets, there exists a positive constant such that

$$|f(x,u,w)| \le M_x \tag{12}$$

for all $(x-x_E) \in \Omega_{\rho*}$, $x_E \in \Gamma$, $u \in U$, and $w \in W$. This can be extended to the deviation system of Eq. (5) given that the rate of change of x_E is bounded

$$|g(x-x_E,x_E,\dot{x}_E,u,w)| \le M \tag{13}$$

for all $(x-x_E) \in \Omega_{\rho*}$, $x_E \in \Gamma$, $u \in U$, and $w \in W$. In addition, by the continuous differentiable property of the Lyapunov function $V(e,x_E)$ and the Lipschitz property assumed for the vector field f, there exist positive constants L_w, L_e, L'_w, L'_e, L'_E, L''_E such that

$$|g(e,x_E,\dot{x}_E,u,w)-g(e',x_E,\dot{x}_E,u,0)| \le L_w|w| + L_e|e-e'|, \tag{14}$$

$$\begin{aligned}&\left|\frac{\partial V(e,x_E)}{\partial e} g(e,x_E,\dot{x}_E,u,w) - \frac{\partial V(e',x'_E)}{\partial e} g(e',x'_E,\dot{x}'_E,u,0)\right| \\ &\quad \le L'_w|w| + L'_e|e-e'| + L'_E|x_E-x'_E| + L''_E|\dot{x}_E-\dot{x}'_E|\end{aligned} \tag{15}$$

for all e, $e' \in \Omega_{\rho*}$, x_E, $x'_E \in \Gamma$, $u \in U$, $w \in W$, $|\dot{x}_E| \le \gamma_E$, and $|\dot{x}'_E| \le \gamma_E$.

Remark 2. For broad classes of nonlinear systems arising in the context of chemical process control applications, quadratic Lyapunov functions using state deviation variables (i.e., $V(x) = (x(t)-x_s)^T P(x(t)-x_s)$) have been widely used and have been demonstrated to yield very good estimates of closed-loop stability regions (see Christofides & El-Farra, 2005 and the references therein). In this work, we extend the quadratic Lyapunov function to the case where instead of a fixed equilibrium x_s a time-varying reference trajectory $x_E(t)$ is used (i.e., $V(e(t),x_E(t)) = e(t)Pe(t)$, where $e(t) = x(t)-x_E(t)$). See the "Application to a chemical process example" section for an example.

Remark 3. Since the Lyapunov function is a function of the deviation variable $e(t)$ and the time-varying state trajectory $x_E(t)$, we must consider the stability region for each fixed $x_E \in \Gamma$ with a given Lyapunov-based controller. The set $\Omega_{\rho*}$ is the set whereby feasibility to drive the system with the Lyapunov-based controller to any $x_E \in \Gamma$ from any deviation $e(t)$ starting inside $\Omega_{\rho*}$ is guaranteed. This set can be estimated in the following way: first, the set Γ is chosen. Second, the stability regions $\Omega_{\rho(x_E)}$ for a sufficiently large number of x_E in the set Γ are estimated. These stability regions $\Omega_{\rho(x_E)}$ can be estimated as the level sets (ideally the largest) of $V(e,x_E)$ for a fixed $x_E \in \Gamma$, where $\dot{V}(e,x_E) < 0$ with the Lyapunov-based controller $h(e,x_E)$. Lastly, we can construct the stability region $\Omega_{\rho*}$ as the intersection of these stability regions.

3. Proposed two-layer control framework

In this section, we introduce the proposed two-layered control framework and prove stability and robustness properties of the closed-loop system.

3.1. Implementation strategy

Economic model predictive control (EMPC) is a process control technique that addresses economic process optimization while accounting for process dynamics. Unlike steady-state economic process optimization, the operating policy computed by the EMPC without a terminal constraint is time-varying. For general time-varying operation, the prediction horizon must be sufficiently large to generate time-varying operating policies that are economically better than steady-state operation (Grüne, 2011). However, the computational time and complexity of such an optimization problem (thousands of decisions variables for large-scale systems) may make it difficult to use EMPC in an on-line fashion to calculate optimal control actions in real-time. To address this issue of computational demand, we propose solving the EMPC optimization problem at the beginning of each operating period in an on-line fashion using real-time state measurements and then, use a conventional MPC to force the process states to follow the economically optimal trajectories for one operating period. The operating period t' is chosen based on the time scale of the process dynamics. While in the lower layer any MPC tracking controller could be used, we implement a Lyapunov-based MPC (LMPC) chosen for its unique stability and robustness properties (see Christofides & El-Farra, 2005; Mhaskar et al., 2005, 2006; Muñoz de la Peña & Christofides, 2008). The proposed two layer control framework is shown in Fig. 1.

The implementation strategy is as follows: at the beginning of the operating period t_k, the upper layer EMPC with sampling period Δ_E and prediction horizon N_E receives state feedback from the process and computes the economically optimal state trajectory of the system by solving an optimization problem. The prediction horizon of the EMPC is chosen to be sufficiently large to cover the operating period and the transition to the next operating period (i.e., $t_{k+N_E}-t_k > t'+\Delta N$ where ΔN is the prediction horizon of the LMPC). From the optimal control inputs computed by the EMPC, the economically optimal process state trajectory is computed from t_k to $t_k+t'+N\Delta$ by recursively solving the nominal system model of Eq. (1) ($w(t) \equiv 0$). Between t_k and t_k+t', the lower layer LMPC works to force the closed-loop process state to track these time-varying trajectories. The

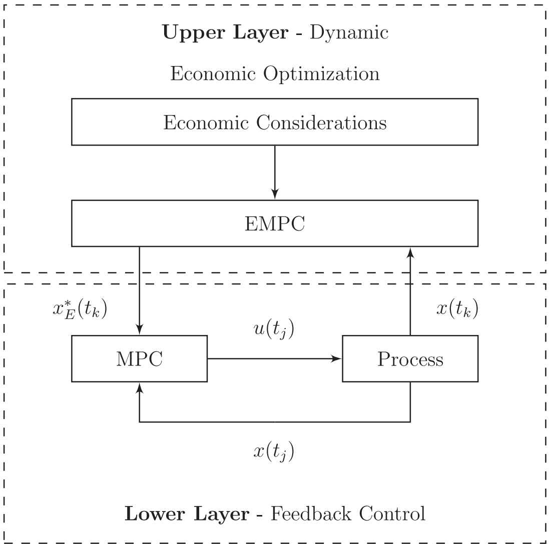

Fig. 1. A block diagram of the proposed dynamic economic optimization and control framework.

addition $N\Delta$ is required because as the end of the operating period approaches, the prediction horizon of the LMPC will extend into the next operating period. Therefore, the LMPC requires a reference trajectory that covers the entire operating period plus the prediction horizon of the LMPC.

The implementation strategy of the proposed dynamic economic optimization and control framework can be summarized as follows:

1. At t_k, the EMPC receives the system state $x(t_k)$ from the sensors and projects the current state $x(t_k)$ onto the set Γ.
2. The EMPC computes the economically optimal state trajectory $x_E^*(t)$ for $t \in [t_k, t_{k+N_E})$.
3. From t_k to $t_k + t'$ (one operating period), the LMPC works to track the economically optimal state trajectory for $t \in [t_k, t_k + t')$.
4. Go to Step 1, $t_k := t_k + t'$.

Remark 4. This control framework is an intermediate approach between existing steady-state operation and one-layer EMPC frameworks that have recently been introduced in the literature. The proposed one-layer EMPCs replace both RTO and the MPC process control layers. With this proposed control framework, any existing MPC systems could be used to track the economically optimal trajectory instead of LMPC.

Remark 5. The operating period t' can be chosen based on the frequency that the process economic information is updated (i.e., energy price, product demand, or product transitions). This operating period is strictly for the purpose of formulating a finite-dimensional optimization problem and should not be considered as a finite operating time as in batch processes since many chemical processes operate continuously for long operating times.

3.2. *Dynamic economic optimization and control framework formulation*

The upper layer EMPC optimization problem of the proposed dynamic economic optimization and control framework for the system of Eq. (1) is as follows:

$$
\begin{aligned}
\underset{u_E \in S(\Delta_E)}{\text{minimize}} \quad & \int_{t_k}^{t_{k+N_E}} L(\tilde{x}_E(\tau), u_E(\tau), \tau)\, d\tau \\
\text{subject to} \quad & \dot{\tilde{x}}_E(t) = f(\tilde{x}_E(t), u_E(t), 0), \\
& u_E(t) \in U, \\
& \tilde{x}_E(t_k) = \underset{\Gamma}{\text{proj}}(x(t_k)), \\
& |\dot{\tilde{x}}_E(t)| \le \gamma_E, \quad \forall t \in [t_k, t_{k+N_E}), \\
& \tilde{x}_E(t) \in \Gamma, \quad \forall t \in [t_k, t_{k+N_E}),
\end{aligned} \tag{16}
$$

where $S(\Delta_E)$ is the family of piece-wise constant functions with sampling period Δ_E, N_E is the prediction horizon of the EMPC, $L(\tilde{x}_E(\tau), u_E(\tau), \tau)$ is the time-dependent economic measure which defines the cost function, the state $\tilde{x}_E$ is the predicted trajectory of the system with manipulated input $u_E(t)$ computed by the EMPC and $x(t_k)$ is the state measurement obtained at time t_k. The optimal solution to this optimization problem, denoted by $u_E^*(t|t_k)$, is defined for $t \in [t_k, t_{k+N_E})$. In the optimization problem of Eq. (16), the first constraint is the nominal model of the system used to predict the future evolution of the process state under sample-and-hold implementation of the EMPC input. The second constraint defines the control energy available to all manipulated inputs. The third constraint defines the initial condition of the optimization problem which is the measurement of the process state at t_k projected onto the set Γ. The fourth constraint limits the rate of change of the economically optimal state trajectory. The fifth constraint ensures that the state evolution is maintained in the region Γ.

The last two constraints of the optimization problem of Eq. (16) are used to guarantee closed-loop stability under this integrated framework and to ensure that the lower layer can force the system to track the state trajectory $x_E^*(t)$. This is a departure from other types of two-layer dynamic economic optimization architectures such as dynamic real-time optimization (D-RTO). The constraint on the rate of change of the economically optimal trajectory does pose a restriction on the feasible set of the optimization problem of Eq. (16) and thus, can affect closed-loop economic performance of the control framework. However, a system that requires a large rate of change on the trajectory $x_E(t)$ to achieve closed-loop economic performance that is better than steady-state may be undesirable for many applications based on practical considerations like excessive strain on control actuators as well as the difficulty of forcing the system to track a rapidly changing operating trajectory in the presence of disturbances.

At the lower process control level, we use LMPC to force the process state to track the economically optimal state trajectory $x_E^*(t)$ obtained by recursively solving the nominal model of Eq. (1) with manipulated input $u_E^*(t)$ applied in a sample-and-hold fashion for $t \in [t_k, t_k + t' + \Delta N)$, where t_k is the beginning of the operating period, t' is the operating period, and ΔN is the prediction horizon of the LMPC. We assume that the LMPC recomputes new manipulated inputs synchronously every Δ and denote the sampling times of the LMPC as $t_j = t_k + j\Delta$, $j = 0, 1, \ldots, t'/\Delta$. We define the system of Eq. (1) in terms of the deviation from the economically optimal state trajectory

$$
e(t) = x(t) - x_E^*(t) \tag{17}
$$

The LMPC at t_j is formulated as

$$
\begin{aligned}
\underset{u \in S(\Delta)}{\text{minimize}} \quad & \int_{t_j}^{t_{j+N}} \left(|\tilde{e}(\tau)|_{Q_c} + |u(\tau) - u_E^*(\tau)|_{R_c} \right) d\tau \\
\text{subject to} \quad & \dot{\tilde{e}}(t) = g(\tilde{e}(t), x_E^*(t), \dot{x}_E^*(t), u(t), 0), \\
& u(t) \in U, \\
& \tilde{e}(t_j) = x(t_j) - x_E^*(t_j),
\end{aligned}
$$

$$\frac{\partial V(e(t_j),x_E^*(t_j))}{\partial e} g(e(t_j),x_E^*(t_j),\dot{x}_E^*(t_j),u(t_j),0) \le \frac{\partial V(e(t_j),x_E^*(t_j))}{\partial e} g(e(t_j),x_E^*(t_j),\dot{x}_E^*(t_j),h(e(t_j),x_E(t_j)),0) \quad (18)$$

where $S(\Delta)$ is the family of piece-wise constant functions with sampling period Δ, N is the prediction horizon of the LMPC, $\tilde{e}(t)$ is the predicted deviation between the state trajectory predicted by the nominal model with manipulated input $u(t)$ computed by the LMPC and the economically optimal state trajectory $x_E^*(t)$. The optimal solution of the optimization problem of Eq. (18) is denoted by $u^*(t|t_j)$ defined for $t \in [t_j,t_{j+N})$. In the optimization problem of Eq. (18), the first constraint is the nominal deviation system of Eq. (5). The second constraint defines the control energy available to all manipulated inputs. The third constraint is the initial condition on the optimization problem. The last constraint ensures that the Lyapunov function of the closed-loop system with LMPC decreases by at least the rate achieved by the Lyapunov-based controller $h(e,x_E)$ when it is implemented in a sample-and-hold fashion.

The manipulated inputs of the proposed control design from time t_j to t_{j+1} are defined as follows:

$$u(t) = u^*(t|t_j), \quad \forall t \in [t_j,t_{j+1}) \quad (19)$$

Remark 6. The third constraint of Eq. (16) may be any projection that projects the current state $x(t_k)$ onto a near (ideally the nearest) state $x_E(t_k)$ in the set Γ. In some cases, when the sampling periods of the upper and lower layers and the bounded disturbance are sufficiently small, it may also be sufficient to use in Eq. (16) the predicted state $\tilde{x}_E(t_k)$ derived from the solution of the optimization problem of Eq. (16) that was previously solved for the preceding operating period.

Remark 7. Because the lower-layer LMPC is based on an explicit Lyapunov-based controller, the LMPC inherits the stability and robustness properties of this explicit controller. This point has been demonstrated many times in our previous work (see, for instance, Muñoz de la Peña & Christofides, 2008 for a thorough discussion of this point).

3.3. Stability analysis

In this subsection, we present the stability properties of the proposed two-layer control framework with the EMPC at the upper layer and the LMPC at the lower layer for the system of Eq. (1). The following proposition proves that the EMPC is a feasible optimization problem and the optimal state trajectory $x_E^*(t)$ is always embedded in the set Γ when $(x(t_k)-x_E(t_k)) \in \Omega_{\rho*}$.

Proposition 1. *Consider the nominal system of Eq. (1) along the prediction horizon under the EMPC design of Eq. (16). Since $x_E(t_k) \in \Gamma$, then the optimization problem of Eq. (16) is feasible and the optimal state trajectory $\tilde{x}_E^*(t)$ computed by applying the optimal manipulated control input $u_E^*(t)$ defined for $t \in [t_k,t_{k+N_E})$ in a sample-and-hold fashion is always embedded in the set Γ.*

Proof. When the EMPC optimization problem of Eq. (16) is solved with an initial condition satisfying $x_E(t_k) \in \Gamma$ (this is guaranteed through the projection procedure), the feasibility of the optimization problem follows because maintaining operation at the initial condition along the predicted horizon (i.e., $\tilde{x}_E(t) = \mathrm{proj}_\Gamma(x(t_k))$ for $t \in [t_k,t_{k+N_E})$) is a feasible solution to the optimization problem as it satisfies all the constraints. Furthermore, the state trajectory $\tilde{x}_E^*(t)$ is always bounded in the set Γ guaranteed through formulation of the optimization problem. □

Theorem 1 provides sufficient conditions such that the LMPC can track the economically optimal trajectory $x_E^*(t)$ with an ultimate bound on the deviation of ϵ_{error}.

Theorem 1. *Consider the system of Eq. (1) in closed-loop under the tracking LMPC of Eq. (18) based on a controller $h(e,x_E)$ that satisfies the conditions of Eqs. (7)–(11). Let $\epsilon_{\text{error}}>0$, $\mu>0$, $\epsilon_w>0$, $\Delta>0$, $\Delta_E>0$, $N \ge 1$, $N_E \ge 1$, $\gamma_E>0$ satisfy*

$$|\dot{x}_E^*(t)| \le \gamma_E < \frac{\hat{\theta}\alpha_3(\epsilon_{\text{error}})}{2L''_E+\alpha_4(\alpha_1^{-1}(\rho^*))+\alpha_5(\alpha_1^{-1}(\rho^*)+M\Delta)}, \quad (20)$$

$$\mu = \alpha_3^{-1}\left[\frac{(2L''_E+\alpha_4(\alpha_1^{-1}(\rho^*))+\alpha_5(\alpha_1^{-1}(\rho^*)+M\Delta))\gamma_E}{\hat{\theta}}\right] < \epsilon_{\text{error}}, \quad (21)$$

$$-(1-\hat{\theta})\alpha_3(\mu)+L'_w\theta+L'_e M\Delta+L'_E\gamma_E\Delta_E \le -\epsilon_w/\Delta \quad (22)$$

for some $\hat{\theta}$ with $0<\hat{\theta}<1$. If $(x(t_0)-x_E(t_0)) \in \Omega_{\rho*}$, then the deviation state $e(t)$ of the closed-loop system is always bounded in $\Omega_{\rho*}$ and the actual closed-loop state trajectory $x(t)$ is always bounded. Furthermore, after some finite time, the deviation between the actual system trajectory of Eq. (1) and that of the economically optimal trajectory $x_E^*(t)$ is ultimately bounded by

$$|e(t)| \le \epsilon_{\text{error}} \quad (23)$$

for $t \in [t_k,t_k+t')$.

Proof. The proof consists of two parts. We first prove that the LMPC optimization problem of Eq. (18) is feasible for all states $(x-x_E) \in \Omega_{\rho*}$. Subsequently, we prove that the deviation between the actual system evolution and the economically optimal trajectory we wish to track is always bounded in $\Omega_{\rho*}$ and the deviation system evolution $e(t)=x(t)-x_E(t)$ is ultimately bounded in $B_{\epsilon_{\text{error}}}$.

Part 1: When the deviation between the actual system trajectory and the economically optimal trajectory $e(t)=x(t)-x_E^*(t)$ is maintained in $\Omega_{\rho*}$ (which will be proved in Part 2), the feasibility of the LMPC of Eq. (18) follows because the input trajectories $u(t)$ such that $u(t)=h(e(t),x_E^*(t))$, $\forall t \in [t_j,t_{j+N})$ are feasible solutions to the optimization problem of Eq. (18) since such trajectories satisfy the input and the Lyapunov function constraints of Eq. (18). This is guaranteed by the closed-loop stability property of the Lyapunov-based controller.

Part 2: We consider the deviation between the actual system trajectory $x(t)$ and the economically optimal trajectory $x_E^*(t)$ which we define as $e(t)=x(t)-x_E^*(t)$. At t_0, the EMPC recomputes a new optimal trajectory $x_E^*(t)$ for the LMPC to track for one operating period from t_0 to t_0+t'. We define two sets $B_{\epsilon_{\text{error}}}=\{|e(t)| \le \epsilon_{\text{error}}\}$ and $B_\mu=\{|e(t)| \le \mu\}$, where μ is defined in Eq. (21) and $B_\mu \subset B_{\epsilon_{\text{error}}}$. For a fixed $x_E \in \Gamma$, the set $B_{\epsilon_{\text{error}}}=\{e(t) \in \Omega_{\rho*}, x_E \in \Gamma \,|\, |x(t)-x_E| \le \epsilon_{\text{error}}\}$. We show that if the deviation between the actual system trajectory and the economically optimal trajectory is in the set $\Omega_{\rho*}\backslash B_\mu$ and the conditions of Eqs. (20) and (21) are satisfied, the Lyapunov function computed along the trajectory of the closed-loop system of Eq. (5) under LMPC will decrease. After some finite time, the deviation will converge to the set B_μ. Furthermore, we show that the deviation $e(t)$ is ultimately bounded in the ball $B_{\epsilon_{\text{error}}}$.

At sampling time $t_j \in [t_0,t_0+t')$ of the LMPC, we assume $e(t_j) \in \Omega_{\rho*}\backslash B_\mu$. The derivative of the Lyapunov function along the deviation system trajectory of Eq. (5) at t_j is

$$\dot{V}(e(t_j),x_E(t_j)) = \frac{\partial V(e(t_j),x_E(t_j))}{\partial e}\dot{e}(t_j) + \frac{\partial V(e(t_j),x_E(t_j))}{\partial x_E}\dot{x}_E(t_j) \tag{24}$$

Substituting $\dot{e}(t_j) = \dot{x}(t_j) - \dot{x}_E(t_j)$ into Eq. (24) and accounting for the Lyapunov-based constraint of Eq. (18), Eq. (24) can be bounded by

$$\begin{aligned}\dot{V}(e(t_j),x_E(t_j)) &= \frac{\partial V(e(t_j),x_E(t_j))}{\partial e}(\dot{x}(t_j) - \dot{x}_E(t_j)) \\ &\quad + \frac{\partial V(e(t_j),x_E(t_j))}{\partial x_E}\dot{x}_E(t_j) \\ &\le \frac{\partial V(e(t_j),x_E(t_j))}{\partial e} g(e(t_j),x_E(t_j),0,h(e(t_j),x_E(t_j)),0) \\ &\quad - \frac{\partial V(e(t_j),x_E(t_j))}{\partial e}\dot{x}_E(t_j) + \frac{\partial V(e(t_j),x_E(t_j))}{\partial x_E}\dot{x}_E(t_j)\end{aligned} \tag{25}$$

Taking into account Eq. (8), Eq. (25) yields

$$\begin{aligned}\dot{V}(e(t_j),x_E(t_j)) &\le -\alpha_3(|e(t_j)|) - \frac{\partial V(e(t_j),x_E(t_j))}{\partial e}\dot{x}_E(t_j) \\ &\quad + \frac{\partial V(e(t_j),x_E(t_j))}{\partial x_E}\dot{x}_E(t_j)\end{aligned} \tag{26}$$

The derivative of the Lyapunov function along the deviation and economically optimal state trajectories for $\tau \in [t_j, t_j + \Delta)$ is given by

$$\dot{V}(e(\tau),x_E(\tau)) = \frac{\partial V(e(\tau),x_E(\tau))}{\partial e}\dot{e}(\tau) + \frac{\partial V(e(\tau),x_E(\tau))}{\partial x_E}\dot{x}_E(\tau) \tag{27}$$

Adding and subtracting $\dot{V}(e(t_j),x_E(t_j))$ of Eq. (24) to/from the right-hand side of Eq. (27) and using the bound of Eq. (26), we have

$$\begin{aligned}\dot{V}(e(\tau),x_E(\tau)) &\le -\alpha_3(|e(t_j)|) + \frac{\partial V(e(\tau),x_E(\tau))}{\partial e}\dot{e}(\tau) \\ &\quad - \frac{\partial V(e(t_j),x_E(t_j))}{\partial e}\dot{e}(t_j) + \frac{\partial V(e(\tau),x_E(\tau))}{\partial x_E}\dot{x}_E(\tau) \\ &\quad - \frac{\partial V(e(t_j),x_E(t_j))}{\partial e}\dot{x}_E(t_j)\end{aligned} \tag{28}$$

From the Lyapunov function constraints of Eqs. (9) and (10), the bound on $\dot{x}_E$, and the Lipschitz property of Eq. (15), Eq. (28) become

$$\begin{aligned}\dot{V}(e(\tau),x_E(\tau)) &\le -\alpha_3(|e(t_j)|) + L'_w|w(\tau)| + L'_e|e(\tau) - e(t_j)| \\ &\quad + L'_E|x_E(\tau) - x_E(t_j)| + L''_E|\dot{x}_E(\tau) - \dot{x}_E(t_j)| \\ &\quad + \alpha_4(|e(t_j)|)\gamma_E + \alpha_5(|e(\tau)|)\gamma_E\end{aligned} \tag{29}$$

Taking into account Eqs. (13) and (3) and the continuity of $e(t)$ and $x_E(t)$, the following bounds can be written for all $\tau \in [t_j, t_{j+1})$

$$|e(\tau) - e(t_j)| \le M\Delta \tag{30}$$

$$|x_E(\tau) - x_E(t_j)| \le \gamma_E \Delta_E \tag{31}$$

From Eq. (30), a bound on $|e(\tau)|$ can obtain

$$|e(\tau)| \le |e(t_j)| + M\Delta \tag{32}$$

Applying Eqs. (30) and (31), the bound on the disturbance $|w(\tau)| \le \theta$, and the bound on $\dot{x}_E$ to Eq. (29) yields

$$\begin{aligned}\dot{V}(e(\tau),x_E(\tau)) &\le -\alpha_3(|e(t_j)|) + L'_w\theta + L'_e M\Delta + L'_E\gamma_E\Delta_E + 2L''_E\gamma_E \\ &\quad + \alpha_4(|e(t_j)|)\gamma_E + \alpha_5(|e(\tau)|)\gamma_E\end{aligned} \tag{33}$$

Accounting for the fact that $e(t_j) \in \Omega_{\rho*} \backslash B_\mu$ and the bound of Eq. (32), the following bound can be written

$$\begin{aligned}\dot{V}(e(\tau),x_E(\tau)) &\le -\alpha_3(\mu) + L'_w\theta + L'_e M\Delta + L'_E\gamma_E\Delta_E \\ &\quad + (2L''_E + \alpha_4(\alpha_1^{-1}(\rho^*)) + \alpha_5(\alpha_1^{-1}(\rho^*) + M\Delta))\gamma_E\end{aligned} \tag{34}$$

If Eq. (20) is satisfied, then there exists a γ_E such that the following holds:

$$\dot{V}(e(\tau),x_E(\tau)) \le -(1-\hat{\theta})\alpha_3(\mu) + L'_w\theta + L'_e M\Delta + L'_E\gamma_E\Delta_E \tag{35}$$

for some positive $\hat{\theta} < 1$. If the condition of Eq. (22) is satisfied, then there exists $\epsilon_w > 0$ such that the following inequality holds for $e(t_j) \in \Omega_{\rho*} \backslash B_\mu$.

$$\dot{V}(e(\tau),x_E(\tau)) \le -\epsilon_w/\Delta, \quad \forall \tau \in [t_j, t_{j+1}) \tag{36}$$

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

$$V(e(t_{j+1}),x_E(t_{j+1})) \le V(e(t_j),x_E(t_j)) - \epsilon_w \tag{37}$$

$$V(e(t),x_E(t)) \le V(e(t_j),x_E(t_j)), \quad \forall t \in [t_j, t_{j+1}) \tag{38}$$

for all $e(t_j) \in \Omega_{\rho*} \backslash B_\mu$. Using the above inequalities recursively, it can be proved that if $e(t_j) \in \Omega_{\rho*} \backslash B_\mu$, the deviation between the actual state trajectory and the economic optimal trajectory converges to B_μ in a finite number of sampling times without going outside the set $\Omega_{\rho*}$. Since the deviation state $e(t)$ is always embedded in the set $\Omega_{\rho*}$ and from Proposition 1, $x_E(t)$ is always embedded in the set Γ, the boundedness of the actual system state trajectory $x(t)$ follows because $\Omega_{\rho*}$ and Γ are compact sets.

To summarize, we proved that if $e(t_j) \in \Omega_{\rho*} \backslash B_\mu$, then

$$V(e(t_{j+1}),x_E(t_{j+1})) \le V(e(t_j),x_E(t_j)) \tag{39}$$

Furthermore, the deviation between the actual state trajectory $x(t)$ and the economic optimal trajectory $x_E(t)$ is ultimately bounded by

$$|e(t)| \le \epsilon_{\text{error}} \tag{40}$$

This statement holds because one can pick a sufficiently large $\epsilon_{\text{error}} > 0$ such that if the deviation comes out of the ball B_μ, the deviation is maintained within the ball $B_{\epsilon_{\text{error}}}$ given that the amount that the deviation can increase over one sampling period is bounded in Eq. (32) and once the deviation comes out of the ball B_μ the Lyapunov function decreases. □

Remark 8. We note that there are essentially four factors influencing the rate of change of the Lyapunov function when $e(t_j) \in \Omega_{\rho*} \backslash B_\mu$ as observed in Eq. (34): the sampling period of the EMPC and LMPC, the bound on the disturbance, and the bound on the rate of change of the economically optimal trajectory. While the bound on the disturbance is a property of the system, two of the other properties can be used to achieve a desired level of tracking for a fixed sampling period of the EMPC: the sampling period of the lower level control loop and the rate of change of the economically optimal tracking trajectory. This relationship is governed by the positive parameter $\hat{\theta} < 1$.

Remark 9. Theorem 1 clarifies how the parameter γ_E arises and why it is needed in the formulation of the EMPC of Eq. (16). We note that γ_E depends on the stability properties and sampling period of the lower level LMPC.

Remark 10. While no guarantee is made that the closed-loop economic performance with the proposed two-layer framework is better compared to using a steady-state model in the upper layer, it may be the case that closed-loop performance is the same or possibly better using a steady-state model in the upper layer EMPC. In this case, the stability result presented here may still be used as long as the conditions are satisfied (i.e., the rate of change of the optimal steady-state varies sufficiently slow). See the "Application to a chemical process example" section for a case where the proposed two-layer dynamic economic optimization and control framework does improve closed-loop economic performance compared to steady-state operation.

Remark 11. We note that both optimization problems of Eqs. (16) and (18) are continuous in time. Numerical methods are required to solve these problems (both integrate the dynamic models and solve the optimization problem). This will lead to discretization error and possibly small constraint violations. In this work, we assume this error is negligible or is sufficiently small such that it can be considered a bounded disturbance. In the "Application to a chemical process example" section, we use an integration step that has been chosen to be significantly smaller than the sampling period of the upper and lower layer such that this discretization error is negligible.

4. Application to a chemical process example

Consider a well-mixed, non-isothermal continuous stirred tank reactor (CSTR) where an elementary reaction takes place of the form $A \to B$. The feed to the reactor consists of pure A at volumetric flow rate F, temperature $T_0+\Delta T_0$ and molar concentration $C_{A0}+\Delta C_{A0}$. A jacket around the reactor is used to provide/remove heat to the reactor. The dynamic equations describing the behavior of the system, obtained through material and energy balances under standard modeling assumptions, are given as

$$\frac{dT}{dt} = \frac{F}{V_R}(T_0+\Delta T_0-T) - \frac{\Delta H k_0}{\varrho c_p} e^{-E/RT} C_A + \frac{Q}{\varrho c_p V_R} \tag{41}$$

$$\frac{dC_A}{dt} = \frac{F}{V_R}(C_{A0}+\Delta C_{A0}-C_A) - k_0 e^{-E/RT} C_A \tag{42}$$

where C_A is the concentration of the reactant A in the reactor, T is the reactor temperature, Q is the rate of heat input/removal, V_R is the reactor volume, ΔH is the heat of the reaction, k_0 and E are the pre-exponential constant and activation energy of the reaction, respectively, c_p and ϱ denote the heat capacity and the density of the fluid in the reactor, respectively. The values of the process parameters are shown in Table 1. The system states are $x = [T \;\; C_A]^T$ and the manipulated inputs are the heat rate $u_1 = Q$ with available control energy $u_1 \in [-2\times 10^5, 2\times 10^5]$ kJ/h and the inlet reactant concentration $u_2 = C_{A0}$ with available control energy $u_2 \in [0.5, 8]$ kmol/m^3. The fluctuation in feed temperature and reactant concentration is considered as a bounded disturbance: Gaussian white noise with zero mean, variances $\sigma_{\Delta T_0} = 20\ \text{K}^2$ and $\sigma_{\Delta C_{A0}} = 0.1\ \text{kmol}^2/\text{m}^6$, and bounds given by $|\Delta T_0| \le 15$ K and $|\Delta C_{A0}| \le 1.0$ kmol/m^3. To simulate the reactor feed disturbances, a new random number is generated and applied over each sampling period.

The control objective is to force the system to track the economically optimal time-varying operating trajectories computed by the upper layer EMPC. We define the set as

$$\Gamma := \{x \in \mathbf{R}^2 \,|\, 340 \le x_1 \le 390\ \text{K}, 0.5 \le x_2 \le 3.0\ \text{kmol/m}^3\} \tag{43}$$

In this example, the economic measure we consider penalizes energy consumption, credits conversion of the reactant to the product, and penalizes the deviation of temperature from 365 K which acts like a safety factor to prevent the system from operating on the boundary of Γ for long periods of time

$$L(x(t),u(t),t) = A_1(t)u_1^2(t) - A_2(t)\frac{(u_2(t)-x_2(t))}{u_2(t)} + A_3(t)(x_1 - 365\ \text{K})^2 \tag{44}$$

where A_1, A_2, and A_3 are the potentially time-varying weighting factors. We chose values of the economic weighting factors so all terms in the economic cost are competitive. For this example, we choose A_1 and A_3 to be time-varying and $A_2 = 10$ to be constant. The time-varying weight $A_1(t)$ is given by

$$A_1(t) = \begin{cases} 1.0\times 10^{-7}, & t < 1.0\ \text{h} \\ 5.0\times 10^{-8}, & 1.0\ \text{h} \le t < 2.0\ \text{h} \\ 1.0\times 10^{-8}, & 2.0\ \text{h} \le t < 3.0\ \text{h} \\ 5.0\times 10^{-8}, & t \ge 3.0\ \text{h} \end{cases}$$

used to model the time-varying energy cost and the time-varying weight $A_3(t)$ is given by

$$A_3(t) = \begin{cases} 1.0\times 10^{-2}, & t < 1.0\ \text{h} \\ 7.5\times 10^{-3}, & 1.0\ \text{h} \le t < 2.0\ \text{h} \\ 5.0\times 10^{-3}, & 2.0\ \text{h} \le t < 3.0\ \text{h} \\ 7.5\times 10^{-3}, & t \ge 3.0\ \text{h} \end{cases}$$

The rationale for varying A_3 is as the energy cost decreases, we penalize the deviation of the temperature less to allow the system to operate closer to the boundary of Γ to take advantage of the decreased energy cost. The EMPC is implemented with a sampling period of $\Delta_E = 36$ s and prediction horizon of $N_E = 60$. It recomputes a new optimal state trajectory at every 0.50 h. The prediction horizon and operating period were chosen to account for the piecewise time-varying energy cost A_1. Since the vector field of the system of Eqs. (41) and (42) is Lipschitz and is input-affine, we use the natural bound of the vector field to bound the rate of change of the time-varying trajectory computed by the EMPC (i.e., γ_E of Eq. (16) is equal to M_x of Eq. (12)). In this two-state example, we define the projection operator of Eq. (16) such that it projects the current state $x(t_k)$ to the closest boundary of Γ if the current state is outside the set Γ (e.g., if $x(t_k) = [400\ \text{K}, 2.0\ \text{kmol/m}^3]$, then $\text{proj}_\Gamma(x(t_k)) = [390\ \text{K}, 2.0\ \text{kmol/m}^3]$).

Remark 12. In practice, the energy weight as well as other time-varying weights for other examples would come from higher level information systems. Here, we assume that we know the weights *a priori*, but this may not be possible for some applications. Instead, we emphasize the importance of choosing the operating period that the EMPC recomputes the optimal economic operating trajectories such that it can account for the update frequency of these weights.

In the lower layer, a tracking LMPC is used to force the system to follow the optimal time-varying reactant concentration trajectory denoted $x_E^*(t)$ computed from the EMPC. To design the LMPC, we define the Lyapunov-based controller $h(x)$ as two proportional controllers given by

$$h(x) = \begin{cases} -K_1(x_1(t) - x_{E,1}^*(t)) + u_{s,1}(t) \\ -K_2(x_2(t) - x_{E,2}^*(t)) + u_{s,2}(t) \end{cases} \tag{45}$$

where $K_1 = 8000$ and $K_2 = 0.01$ and u_s is the steady-state input corresponding to the steady-state $x_E^*(t)$ (i.e., the input vector that makes the right-hand side of Eqs. (41) and (42) equal to zero with the state vector x_E^*). We define a quadratic Lyapunov function of form $V(e, x_E) = e^T P e$ with

$$P = \begin{bmatrix} 10 & 1 \\ 1 & 100 \end{bmatrix} \tag{46}$$

is used. The LMPC is implemented with a sampling time $\Delta = 36$ s, prediction horizon $N=5$, and weighting matrices of $Q_c = P$ and

Table 1
Process parameters.

F	5.0	m^3/h	ΔH	-1.2×10^4	kJ/kmol
V_R	1.0	m^3	k_0	3×10^7	h^{-1}
T_0	300	K	E	5×10^4	kJ/kmol
C_{A0}	4	kmol/m^3	ϱ	1000	kg/m^3
R	8.314	kJ/kmol K	c_p	0.231	kJ/kg m^3

$R_c = \text{diag}[10^{-7} \;\; 10]$. The sampling time was chosen to be the same as the EMPC so that the trajectory $x_E^*(t)$ could be sent directly down from the EMPC and did not need to be recomputed with the time partitioning of the LMPC. While in this example we have chosen the sampling times to be the same for both the LMPC and EMPC, this is not necessary. The prediction horizon and weighting matrices were chosen to achieve a close tracking of the optimal state trajectory.

With the given nonlinear system of Eqs. (41) and (42), Lyapunov-based controller, and Lyapunov function the stability regions of the closed-system with the Lyapunov-based controller can be estimated for a sufficiently large number of fixed $x_E \in \Gamma$. After this is completed, we take the intersection of all the stability regions to estimate the closed-loop stability region $\Omega_{\rho*}$ of the system with the Lyapunov-based controller. In this example, $\Omega_{\rho*}$ is estimated to be $\rho^* = 110$. Through the Lyapunov-based constraint on the LMPC of Eq. (18), the closed-loop system with the proposed two-layer framework inherits this stability region $\Omega_{\rho*}$.

To simulate the closed-loop system, explicit Euler method with integration step 0.36 s was used to integrate the ODEs and the open source interior point solver Ipopt (Wächter & Biegler, 2006) was used to solve the optimization problems. In a set of closed-loop simulations, we first demonstrate the stability properties of the closed-loop system under the two-layer dynamic economic optimization and control framework. Second, we demonstrate the time-varying operation with the proposed two-layer dynamic economic optimization and control framework. Third, we compare the closed-loop economic performance of the proposed framework compared to using a steady-state model in the upper layer instead of a dynamic model.

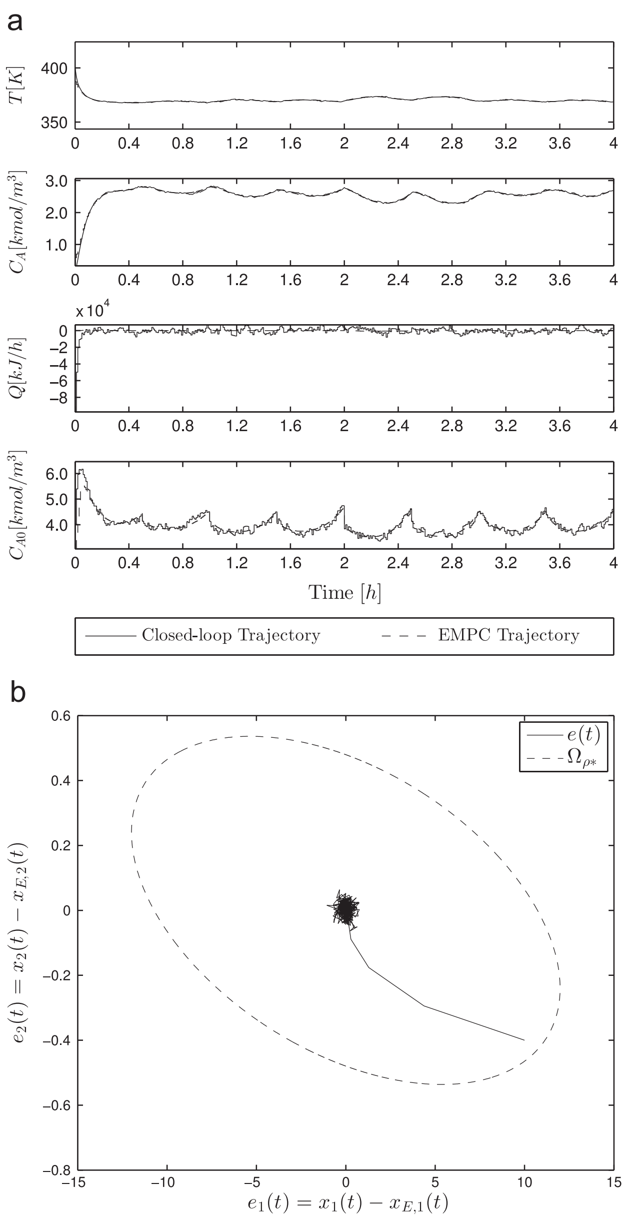

Fig. 2. The closed-loop system states and inputs of Eqs. (41) and (42) with feed disturbance and starting from 400 K and 0.1 kmol/m^3 plotted (a) with time and (b) in deviation state-space.

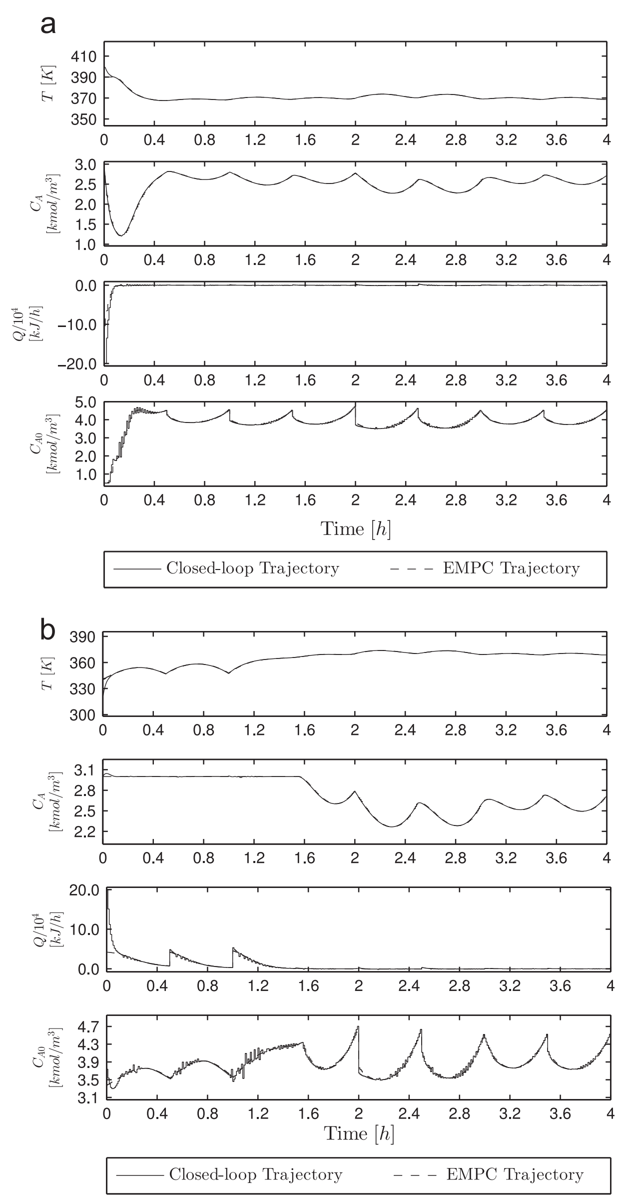

Fig. 3. The closed-loop system states and inputs of Eqs. (41) and (42) without feed disturbance and starting from: (a) 400 K and 3.0 kmol/m^3 and (b) 320 K and 3.0 kmol/m^3.

To demonstrate the closed-loop stability properties of the proposed two-layer framework, we initialize the system at $x_0 = [400\ \text{K}, 0.1\ \text{kmol/m}^3]$ which is outside of Γ, but inside the stability region $\Omega_{\rho*}$. The projection operator of the upper layer EMPC projects this initial state onto the state $x_{E,0} = [390\ \text{K}, 0.5\ \text{kmol/m}^3] \in \Gamma$ to use as an initial condition to the optimization problem of Eq. (16). The evolution of the closed-loop system with the proposed two-layer framework and with the inlet temperature and reactant concentration disturbance added is plotted in Fig. 2. From Fig. 2b, the deviation of the actual system state and the economically optimal state are always maintained inside $\Omega_{\rho*}$ and become small after some finite time.

Two simulations of the closed-loop system without feed disturbance are plotted in Fig. 3 with two different initial conditions to demonstrate the time-varying operation with the proposed two-layer dynamic economic optimization and process control framework. The system state in Fig. 3(a) starts from the initial temperature 400 K and initial concentration 3.0 kmol/m^3 and the system state in Fig. 3(b) starts from initial temperature 320 K and initial concentration 3.0 kmol/m^3. Initially, the closed-loop evolution of the two simulations are different. The simulation starting at the larger temperature must remove heat while not supplying much reactant material to the reactor to reduce the reactor temperature. In contrast, the simulation that starts at the smaller temperature must supply heat and reactant material to the reactor to increase the reactor temperature. After a long enough operation of the reactor, the effect of the initial condition diminishes and the closed-loop time-varying evolution of the two simulations becomes similar, but the reactor is still operated in a time-varying fashion.

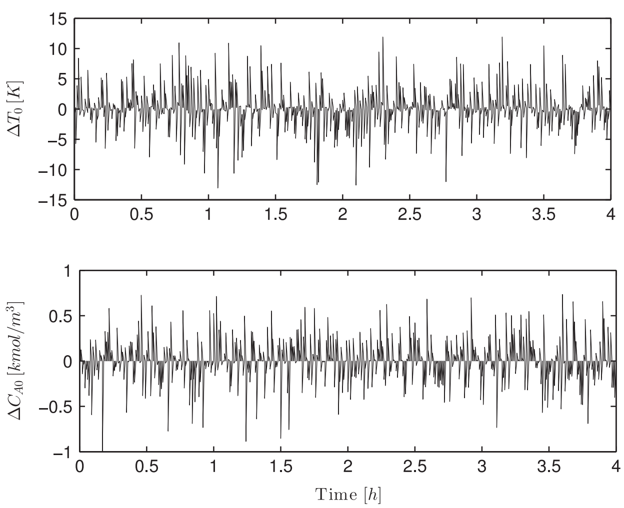

Fig. 4. The process feed disturbance noise realization applied to the closed-loop systems simulated with feed temperature and reactant concentration disturbances.

To compare the closed-loop economic performance under the proposed dynamic economic optimization and control framework and steady-state operation, we define the total economic cost over the simulation as

$$\tilde{J}_E = \sum_{j=0}^{M} \left(A_1(t_j)Q^2(t_j) + A_2 \frac{C_A(t_j)}{C_{A0}(t_j)} + A_3(T(t_j) - 365\ \text{K})^2 \right) \tag{47}$$

where t_0 is the initial time of the simulation and $t_M = 4.0$ h is the end of the simulation. The optimal steady-state from steady-state economic process optimization is

$$x_s^*(t) = \begin{cases} [370.0\ \text{K}, 2.576\ \text{kmol/m}^3]^T, & t < 1.0\ \text{h} \\ [371.7\ \text{K}, 2.447\ \text{kmol/m}^3]^T, & 1.0\ \text{h} \le t < 2.0\ \text{h} \\ [375.2\ \text{K}, 2.205\ \text{kmol/m}^3]^T, & 2.0\ \text{h} \le t < 3.0\ \text{h} \\ [371.7\ \text{K}, 2.447\ \text{kmol/m}^3]^T, & t \ge 3.0\ \text{h} \end{cases}$$

with the corresponding steady-state input of

$$u_s^*(t) = \begin{cases} [0.0\ \text{kJ/h}, 3.923\ \text{kmol/m}^3]^T, & t < 1.0\ \text{h} \\ [-0.5\ \text{kJ/h}, 3.827\ \text{kmol/m}^3]^T, & 1.0\ \text{h} \le t < 2.0\ \text{h} \\ [0.0\ \text{kJ/h}, 3.653\ \text{kmol/m}^3]^T, & 2.0\ \text{h} \le t < 3.0\ \text{h} \\ [-0.5\ \text{kJ/h}, 3.827\ \text{kmol/m}^3]^T, & t \ge 3.0\ \text{h} \end{cases}$$

We implement an LMPC, to drive the system to the time-varying optimal steady-state, which is formulated as follows:

$$\begin{aligned} \underset{u \in S(\Delta)}{\text{minimize}} \quad & \int_{t_j}^{t_{j+N}} \left(|\tilde{x}(\tau) - x_s^*(\tau)|_{Q_c} + |u(\tau) - u_s^*(\tau)|_{R_c} \right) d\tau \\ \text{subject to} \quad & \dot{\tilde{x}}(t) = f(\tilde{x}(t), u(t), 0), \\ & \tilde{x}(t_j) = x(t_j), \\ & -2 \times 10^5 \le u_1(t) \le 2 \times 10^5, \quad \forall t \in [t_j, t_{j+N}), \\ & 0.5 \le u_2(t) \le 8, \quad \forall t \in [t_j, t_{j+N}), \\ & \frac{\partial V(x(t_j))}{\partial x} f(x(t_j), u(t_j), 0) \\ & \le \frac{\partial V(x(t_j))}{\partial x} f(x(t_j), h(x(t_j), x_s^*(t_j)), 0) \end{aligned} \tag{48}$$

Table 2
Total economic cost, given by Eq. (47), comparison for 4 h simulations of the closed-loop system with and without feed disturbance.

Initial conditions		Total economic cost					
$T(t_0)$ (K)	$C_A(t_0)$ (kmol/m^3)	Steady-state optimization without disturbance	EMPC/LMPC without disturbance	Cost decrease (%)	Steady-state optimization with disturbance	EMPC/LMPC with disturbance	Cost decrease (%)
400.0	3.0	21,970.5	14,531.1	51.2	21,642.4	14,130.7	53.2
380.0	3.0	5235.4	3409.5	53.6	5060.1	3037.9	66.6
360.0	3.0	4261.8	3308.6	28.8	4083.2	2997.1	36.2
340.0	3.0	13,732.2	10,997.3	24.9	13,554.9	10,882.3	24.6
320.0	3.0	23,719.4	19,315.9	22.8	23,729.1	19,210.3	23.5
400.0	2.5	18,546.8	10,062.1	84.3	18,283.4	9691.4	88.7
380.0	2.5	4558.7	3163.3	44.1	4387.2	2811.9	56.0
360.0	2.5	4496.4	3335.6	34.8	4322.7	3030.3	42.6
340.0	2.5	14,078.3	11,034.4	27.6	13,910.2	10,928.8	27.3
320.0	2.5	24,052.2	19,293.4	24.7	24,002.2	19,193.8	25.1
400.0	2.0	14,831.5	6774.0	118.9	14,682.4	6412.6	129.0
380.0	2.0	4073.2	3085.1	32.0	3905.0	2739.8	42.5
360.0	2.0	4765.4	3431.2	38.9	4596.4	3139.3	46.4
340.0	2.0	14,395.5	11,162.3	29.0	14,236.8	11,068.2	28.6
320.0	2.0	24,202.7	19,241.2	25.8	24,223.5	19,146.7	26.5
400.0	0.1	8146.1	4360.5	86.8	7999.4	4025.7	98.7

where the Lyapunov function, the Lyapunov-based controller, the weighting matrices R_c and Q_c, the sampling period Δ, and the prediction horizon N are all the same as the ones used in the tracking LMPC scheme. To make a fair comparison with process feed disturbance, the same process noise plotted in Fig. 4 was applied to each closed-loop system simulation with disturbances in feed temperature and reactant concentration. The total economic cost of several closed-loop simulations starting from different initial conditions is shown in Table 2. From the results of Table 2, the largest economic cost decrease occurs for systems starting from higher temperature. When the system starts from a lower temperature, it requires much more heat energy supplied to the reactor initially compared to the heat removed initially when the system starts at a higher temperature as explained above and demonstrated in Fig. 3. Thus, a system starting from a higher temperature is capable of more economic cost reduction because it can use less input heat energy.

5. Conclusions

In this work, we proposed a two-layer framework for integrating dynamic economic optimization and model predictive control for nonlinear process systems. In the upper layer, EMPC is used to compute economically optimal time-varying operating trajectories while restricting the rate of change of the trajectory and constraining the trajectory inside the equilibrium manifold of the process for the allowable values of the control actions. The lower layer model predictive controller designed via Lyapunov-based techniques, is used to force the system to track the optimal time-varying trajectory computed by the EMPC. We proved that the deviation between the actual closed-loop system and the economically optimal closed-loop trajectory is bounded and the closed-loop system state always remains bounded. The theoretical results were demonstrated through a chemical process example.

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