Integrating Dynamic Economic Optimization and Model Predictive Control for Optimal Operation of Nonlinear Process Systems

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OUTLINE

- Background on the integration of economic optimization and process control
- Review of time-varying chemical process operation
- Lyapunov-based model predictive control (MPC) for nonlinear systems
- Proposed two-layer dynamic economic optimization and control framework
  - ◇ Upper-layer Economic MPC (EMPC) formulation
  - ◇ Lower-layer Lyapunov-based MPC (LMPC) formulation
  - ◇ Closed-loop stability analysis
- Application to a chemical process
  - ◇ Achieving practical closed-loop stability
  - ◇ Closed-loop performance evaluation

BACKGROUND

- Model predictive control
  - ◇ Ability to optimally control MIMO systems
  - ◇ Accounts for input and state constraints
  - ◇ Quadratic cost function penalizing deviation of states and inputs from economically optimal steady-states typically used
- Economic optimization of chemical processes via real-time optimization (RTO)

  (TE. Marlin *et al.*, *AIChE Symposium*, 1997)
  - ◇ Upper layer: Optimizes process operation steady-states via steady-state model for economically optimal operation
  - ◇ Lower layer: Feedback control to force the system to operate at steady-states
- Calls for integrating economic optimization with MPC
  - ◇ Integrating steady-state optimization directly in MPC (M. Tvrzská de Gouvêa *et. al.*, *Comp. & Chem. Eng.*, 1998; C. Yousfi *et. al.*, *ACC*, 1991; A. C. Zanin *et. al.*, *CEP*, 2002)
  - ◇ Use of dynamic model in RTO (D-RTO) (J. V. Kadam *et. al.*, *CAPO*, 2003; X. Zhu *et. al.*, *IEEE IES*, 2004)

BACKGROUND

- One-layer MPC with cost accounting directly for economic considerations (EMPC)
  - ◇ Stability using a suitable Lyapunov function and a terminal constraint (M. Diehl et. al. , *IEEE TAC*, 2011; J. Rawlings *et. al.*, *LNCIS*, 2009)
  - ◇ Economic MPC designed via Lyapunov-based techniques (M. Heidarinejad *et. al.*, *AIChE*, 2012; X. Chen *et. al.*, *JPC*, 2012)
  - ◇ Economic MPC of cyclic processes (R. Huang *et. al., JPC, 2011)*
- Motivating factors for a two-layer approach to integrating economic optimization and process control
  - ◇ Industrial applications would require a complete redesign of control architecture to implement proposed one-layer EMPCs
  - ◇ Most two-layer D-RTO and MPC systems lack a rigorous theoretical treatment of such two layer frameworks
  - ◇ EMPC may require a large prediction horizon making it difficult to solve in real-time

TIME-VARYING / TRANSIENT OPERATION WITHIN CHEMICAL PROCESS OPERATIONS

- Economic MPC operates systems in a time-varying fashion to optimize an economic measure (i.e., as in Model 1 operation in (M. Heidarinejad *et. al.*, *AIChE*, 2012))
- Reasons for time-varying operation of a chemical process:
  1. Explicit time dependence of economic objectives and constraints
  2. Inherent properties of a chemical process
- Examples of time-dependent economic objectives and constraints
  - ◇ Energy cost
  - ◇ Feedstock price or variability
  - ◇ Demand
  - ◇ Product or grade transitions
  - ◇ Product price variability
  - ◇ Material availability

TIME-VARYING / TRANSIENT OPERATION WITHIN CHEMICAL PROCESS OPERATIONS

- Periodically operated reactor examples (H. Budman *et. al.*, *CES*, 2007)
  - ◇ Catalytic packed beds
  - ◇ Continuously stirred tank reactors (with second-order reactions)
  - ◇ Polymerization reactors
  - ◇ Catalytic trickle bed reactors
  - ◇ Simulated moving bed chromatographic systems
  - ◇ Pressure swing adsorption systems
- Techniques exist to identify processes that benefit from periodic operation
  - ◇ Frequency response techniques (J.M. Douglas, *I&EC Process Des. & Dev.*, 1967)
  - ◇ Π-Criterion for identifying CSTR systems that can benefit from forced periodic operation (L.E. Sterman *et. al.*, *AIChE Journal*, 1991)

OPTIMAL TIME-VARYING / TRANSIENT OPERATION WITH ECONOMIC MPC

- Most of the time-varying operation strategies are *ad hoc* (not necessarily the globally optimal operating strategy or even optimal at all)

- EMPC is systematic and able to determine, *in real-time*, the optimal time-varying operating strategies

- EMPC can account for

  - ◇ Time-dependent economic objectives and constraints

  - ◇ State and input constraints

  - ◇ Bounded disturbance attenuation through feedback

  - ◇ Intrinsic properties of systems that benefit from time-varying operation

CLASS OF NONLINEAR SYSTEMS

(M. Ellis *et al.*, *Control Engineering Practice*, submitted, 2012)

- System description

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

◇ $x(t) \in \mathbf{R}^{n_x}$: state of the system

◇ $u(t) \in U \subset \mathbf{R}^{n_u}$: manipulated inputs with $|u_i| \leq u_i^{\max}$ $(i = 1, \ldots, n_u)$

◇ $w(t) \in W$: bounded disturbance

$$W := \{w \in \mathbf{R}^{n_w} \mid |w| \leq \theta, \theta > 0\}$$

◇ f: locally Lipschitz vector function

SYSTEM IN DEVIATION VARIABLE FORM

- Error of system state from EMPC computed optimal operating trajectory

$$e(t) \triangleq x(t) - x_E(t)$$

  - ◇ $x_E(t) \in \Gamma \subset \mathbf{R}^{n_x}$: Reference state trajectory
  - ◇ $e(t) \in \mathbf{R}^{n_x}$: State deviation between the actual trajectory and the reference trajectory

- System dynamics in deviation variable form:

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

- New system has an isolated equilibrium at the origin for each fixed $x_E \in \Gamma$

$$g(0, x_E, 0, u_E, 0) = 0$$

STABILITY ASSUMPTION

- There exists a Lyapunov-based controller, $u = h(e, x_E)$ and a Lyapunov function $V(x)$ such that:

$$\alpha_1(|e|) \leq V(e, x_E) \leq \alpha_2(|e|),$$

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

$$\left| \frac{\partial V}{\partial e} \right| \leq \alpha_4(|e|),$$

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

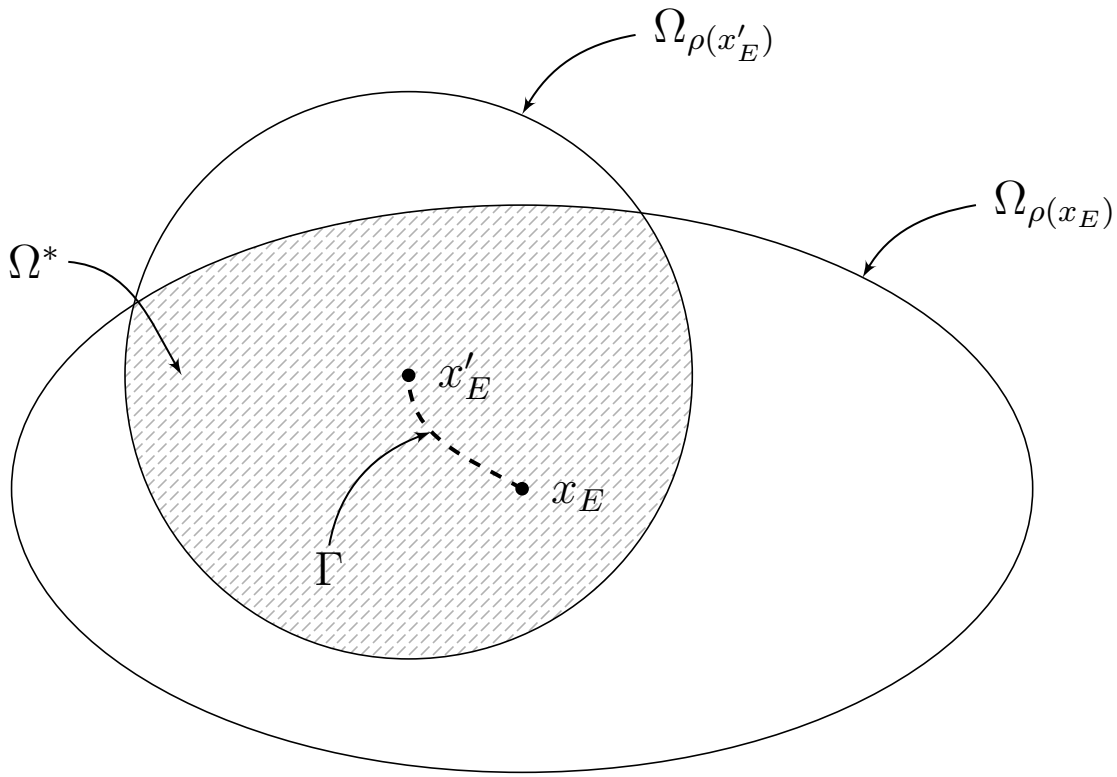
$$h(e, x_E) \in U$$

  for all $e \in D_s \subseteq \mathbf{R}^{n_x}$ (D_s is an open neighborhood of the origin)

- Renders the origin $e = 0$ of the nominal closed-loop system asymptotically stable for each fixed $x_E \in \Gamma$

- Lyapunov-based controller design techniques (P. D. Christofides and N. H. El-Farra, *Springer-Verlag*, 2005; P. Kokotović and M. Arcak, *Automatica*, 2001; Y. Lin and E. D. Sontag, *SCL*, 1990)

STABILITY REGION



- Stability region of the closed-loop system under the Lyapunov-based controller $h(e, x_E)$ for each fixed equilibrium $x_E \in \Gamma$
- $\Omega_{\rho(x_E)}$ can be explicitly characterized for a given controller, system, and fixed $x_E \in \Gamma$
- Denote Ω^* as the intersection of stability regions $\Omega_{\rho(x_E)}$, $x_E \in \Gamma$

LYAPUNOV-BASED MPC

- Lyapunov-based MPC (LMPC)

$$\min_{u \in S(\Delta)} \int_{t_k}^{t_{k+N}} [\tilde{x}(\tau)^T Q_c \tilde{x}(\tau) + u(\tau)^T R_c u(\tau)] d\tau$$

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

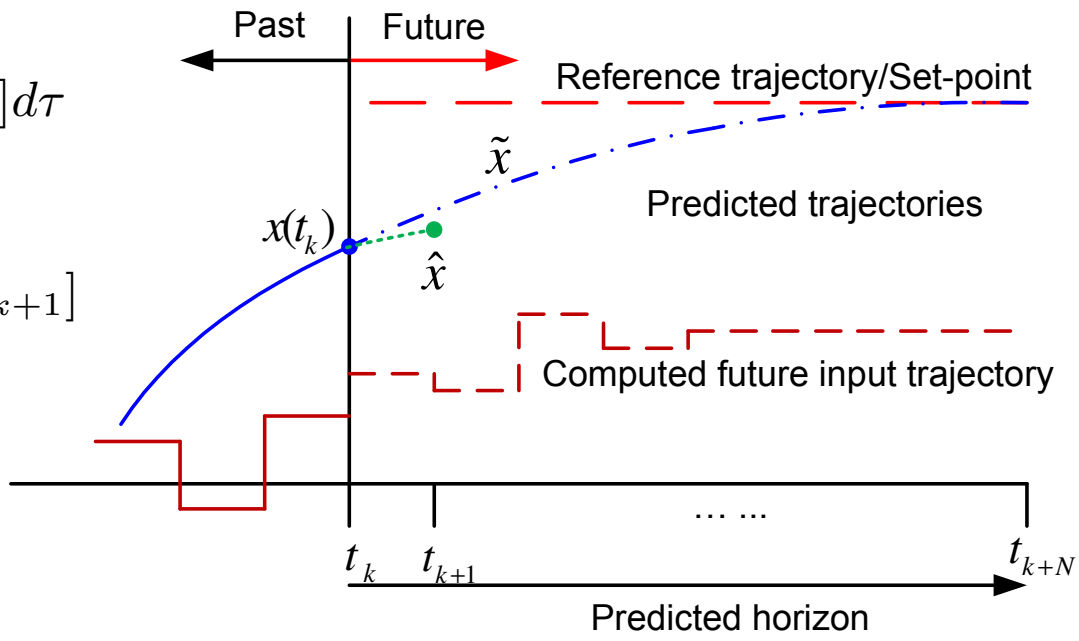
$$\dot{\hat{x}}(t) = f(\hat{x}(t), h(\hat{x}(t_k)), 0), \ t \in [t_k, t_{k+1}]$$

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

$$u(t) \in U$$

$$\tilde{x}(t) \in X$$

$$V(\tilde{x}(t)) \leq V(\hat{x}(t)), \ \forall t \in [t_k, t_{k+1}]$$



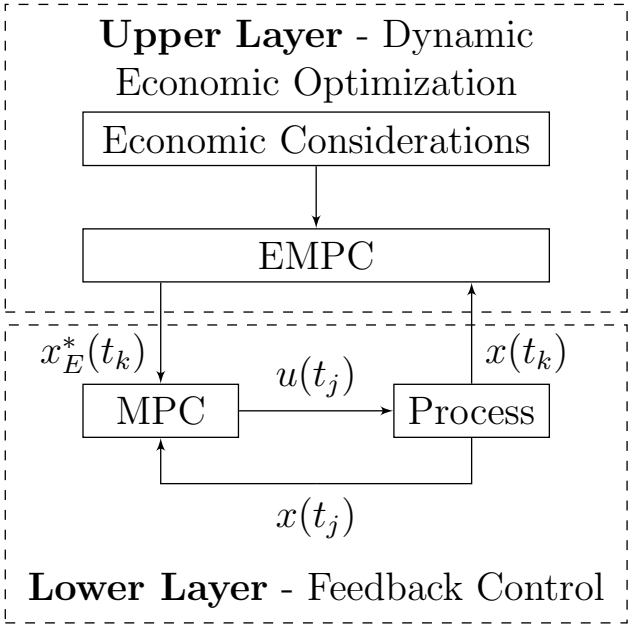
- Guaranteed stability of the closed-loop system (P. Mhaskar *et al.*, *IEEE TAC, 2005; Christofides, Liu and Muñoz de la Peña, Springer, 2011)*
  - ◇ Convergence is guaranteed by the stability constraint
  - ◇ Recursive feasibility is guaranteed by $h(x)$ for all $x \in \Omega_\rho$
- The LMPC inherits the stability properties and the stability region (i.e., Ω_ρ) of the controller $h(x)$ - applied in sample and hold (practical stability)

PROPOSED TWO-LAYER DYNAMIC ECONOMIC OPTIMIZATION AND CONTROL FRAMEWORK

- Conventional MPC
  - ◇ Quadratic cost function for MPC (Q, R: positive definite matrices)
  - ◇ Set-point computation $(x_{\text{set}}, u_{\text{set}})$ via steady-state process model
- Economic MPC
  - ◇ General time-dependent cost function $J = \int_0^{N\Delta} L(x(\tau), u(\tau), \tau) d\tau$
  - ◇ Leads to time-varying process operation
  - ◇ The prediction horizon must be sufficiently large for time-varying operation with EMPC
  - ◇ Key ideas for our approach:
    - ▷ EMPC solved on-line, but outside the feedback control loop
    - ▷ EMPC with sampling period Δ_E resolves the optimization problem every operating period t' using state feedback
    - ▷ Explicit constraints on the EMPC are given to guarantee feasibility of the lower feedback control layer

PROPOSED TWO-LAYER DYNAMIC ECONOMIC OPTIMIZATION AND CONTROL FRAMEWORK

- Block diagram:



- EMPC with sampling period Δ_E recomputes the optimal trajectory every operating period $t' \gg \Delta_E$
- MPC with sampling period Δ recomputes the optimal manipulated input trajectory every $t_j = t_0 + j\Delta$

IMPLEMENTATION STRATEGY

1. At t_k, the EMPC receives the system state $x(t_k) \in \Omega^*$ from the sensors and time-dependent economic information from higher level information systems.

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 MPC works to track the economically optimal state trajectory for $t \in [t_k, t_k + t')$.

4. Go to Step 1, $t_k := t_k + t'$.

UPPER-LAYER EMPC FORMULATION

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

- Constraint (a) and (b) are used to guarantee the lower layer LMPC optimization problem is feasible and can track the state trajectory $x_E(t)$
  - ◇ Constraint (a) - bounds the rate of change of the economically optimal state trajectory
  - ◇ Constraint (b) - restricts the trajectory inside the stability region

LOWER-LAYER LMPC FORMULATION

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

- Use LMPC to take advantage of its unique feasibility and closed-loop stability properties
- Could use any type of MPC to force the system to track the economically optimal state trajectory

STABILITY ANALYSIS

Theorem 1 *Consider the system in closed-loop under the tracking LMPC based on a controller a Lyapunov-based controller $h(e, x_E)$. Let $\epsilon_w > 0$, $\Delta > 0$, $\gamma_E > 0$ satisfy*

$$|\dot{x}_E^*(t)| \leq \gamma_E < \frac{\hat{\theta}\alpha_3(\mu)}{2L_E'' + \alpha_4(\epsilon_{error}) + \alpha_5(\epsilon_{error})},$$

$$-(1-\hat{\theta})\alpha_3(\mu) + L_w'\theta + L_e' M\Delta + L_E' M_E \Delta_E \leq -\epsilon_w/\Delta$$

for some $\hat{\theta}$ with $0 < \hat{\theta} < 1$. If $x(t_0) \in \Gamma$, then the state $x(t)$ of the closed-loop system is always bounded in Ω^* and the deviation between the actual system trajectory and that of the economically optimal trajectory $x_E^*(t)$ is bounded

$$|e(t)| \leq \epsilon_{error}$$

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

- Feasiblity through the Lyapunov-based controller $h(e, x_E)$
- Factors on ϵ_{error}
  1. Sampling periods of the EMPC and LMPC
  2. Bound on the rate of change of the economically optimal trajectory
  3. Bound on the disturbances

APPLICATION TO A CHEMICAL PROCESS

- A well-mixed, non-isothermal CSTR where an elementary reaction takes place of the form $A \rightarrow B$

$$\frac{dT}{dt} = \frac{F}{V}(T_0 + \Delta T_0 - T) - \frac{\Delta H k_0}{\sigma c_p} e^{\frac{-E}{RT}} C_A + \frac{Q}{\sigma c_p V_r}$$
$$\frac{dC_A}{dt} = \frac{F}{V}(C_{A0} + \Delta C_{A0} - C_A) - k_0 e^{\frac{-E}{RT}} C_A$$

- The manipulated input is the external heat input/removed with $|u| \leq 2 \times 10^5\, kJ/h$

- Bounded reactor feed disturbances (modeled as Gaussian white noise)

  - ◇ Feed temperature ΔT_0: variance $\sigma_{\Delta T_0} = 20\, K^2$ and $|\Delta T_0| \leq 20\, K$

  - ◇ Feed reactant concentration ΔC_{A0}: variance $\sigma_{\Delta C_{A0}} = 1\, kmol^2/m^3$ and $|\Delta C_{A0}| \leq 1\, kmol/m^3$

APPLICATION TO A CHEMICAL PROCESS

- **Control Objective:** track the economically optimal time-varying operating trajectories computed by the upper layer EMPC
- Economic cost function accounts for energy efficiency and downstream separations of the reactant from the product

$$L(x(t), u(t), t) = A_1(t)\frac{|u(t)|}{u_{\max}} + A_2(t)\frac{x_2(t)}{C_{A0}}$$

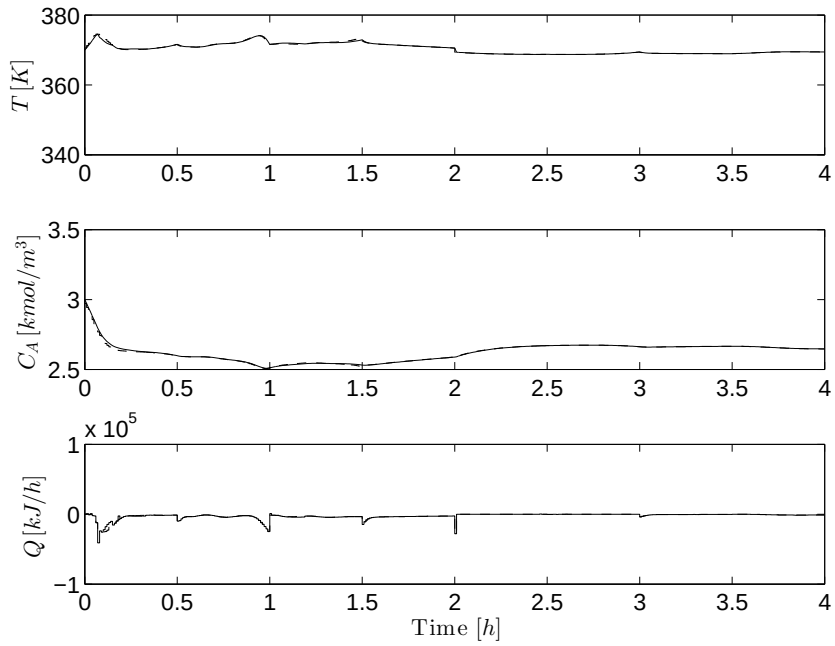
  - ◇ $A_1(t)$, $A_2(t)$ are the potentially time-varying weighting factors
  - ◇ For this work, $A_1(t)$ is time-dependent and A_2 constant with $A_2/C_{A0} = 1$

$$\frac{A_1(t)}{u_{\max}} = \begin{cases} 1 \times 10^{-5}, & t < 1.0\,h \\ 3 \times 10^{-5}, & 1.0\,h \leq t < 2.0\,h \\ 8 \times 10^{-5}, & 2.0\,h \leq t < 3.0\,h \\ 3 \times 10^{-5}, & t \geq 3.0\,h \end{cases}$$

CONTROLLER DESIGN AND PARAMETERS

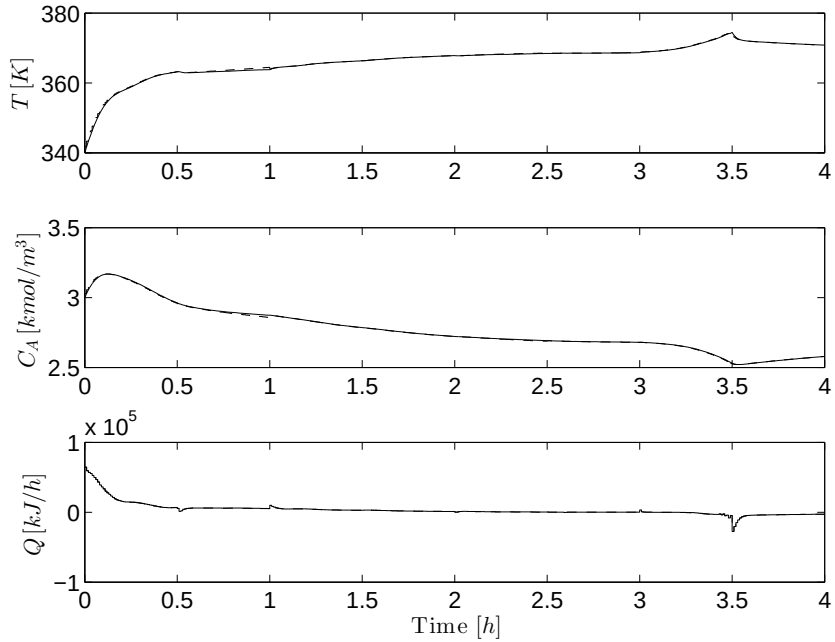
- Lyapunov-based controller designed by Sontag controller (E. D. Sontag, *SCL*, 1989)
- Lyapunov function $V(e, x_E) = e^T P e$ with $P = \text{diag}\begin{bmatrix} 1 & 800 \end{bmatrix}$
- Upper layer EMPC
  - ◇ $\Delta_E = 36\, sec$, $N_E = 125$
  - ◇ Recomputes a new optimal state trajectory every $0.50\, h$
- Lower layer LMPC
  - ◇ Works to track the economically optimal reactant concentration $x^*_{E2}(t)$
  - ◇ $\Delta = 36\, sec$, $N = 5$, $Q_c = 800$, $R_c = 1 \times 10^{-8}$

NOMINAL OPERATION $(T(0), C_A(0)) = (370\,K, 3\,kmol/m^3)$



- Closed-loop system evolution:
  - ◇ Initially, the optimal operating strategy is to allow reaction consume the reactant without supplying/removing heat to/from reactor
  - ◇ Reactor temperature increases and heat is removed to cool reactor
  - ◇ Time-varying operation
- Achieves practical closed-loop stability
- Economic cost improvement of 7.51% compared to steady-state operation

NOMINAL OPERATION $(T(0), C_A(0)) = (340\,K, 3\,kmol/m^3)$



- Closed-loop system evolution:
  - ◇ Initially, the optimal operating strategy is to supply heat to the reactor
  - ◇ Reactor temperature increases and the reactant concentration decreases
  - ◇ Time-varying operation
- Achieves practical closed-loop stability
- Economic cost improvement of 2.24% compared to steady-state operation

CONCLUSIONS

- Proposed a two-layer framework for integrating dynamic economic optimization and model predictive control for nonlinear process systems
  - ◇ Upper layer: EMPC used to compute the economically optimal time-varying operating trajectories
    - ▷ Restricts rate of change of the trajectory
    - ▷ Bounds the trajectory inside the stability region
  - ◇ Lower layer: LMPC designed via Lyapunov-based techniques
- Application to a chemical process
  - ◇ Achieves closed-loop stability
  - ◇ Economic cost improvement for several closed loop simulations

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