8-2018

# Economic Model Predictive Control Design via Nonlinear Model Identification

Laura Giuliani
*University of Study of L'Aquila*

Helen Durand
*Wayne State University*, helen.durand@wayne.edu



## Recommended Citation

Giuliani, L. and H. Durand, "Economic Model Predictive Control Design via Nonlinear Model Identification," *Proceedings of the 6th IFAC Conference on Nonlinear Model Predictive Control*, 6 pages, Madison, Wisconsin, 2018.

# Economic Model Predictive Control Design via Nonlinear Model Identification ⋆

**Laura Giuliani** * **Helen Durand** **

* *Department of Industrial and Information Engineering and Economics, University of Study of L'Aquila, L'Aquila 67100, Italy.*
** *Department of Chemical Engineering and Materials Science, Wayne State University, Detroit, MI 48202, USA (e-mail: helen.durand@wayne.edu)*

**Abstract:** Increasing pushes toward next-generation/smart manufacturing motivate the development of economic model predictive control (EMPC) designs which can be practically deployed. For EMPC, the constraints, objective function, and accuracy of the state predictions would benefit from process models that describe the process physics. However, obtaining first-principles models of chemical process systems can be time-consuming or challenging such that it is preferable to develop physics-based process models automatically from process operating data. In this work, we take initial steps in this direction by suggesting that because experiments that are used to characterize first-principles models often target specific types of data, an EMPC may be utilized to gather non-routine operating data that ideally provides insights on the process physics and thereby allows physics-based process models to be developed on-line. These models can then be used to update the model, objective function, and constraints of the controller. Closed-loop stability and recursive feasibility considerations are discussed for the proposed EMPC design, and the controller's application is illustrated through a chemical process example.

*Keywords:* Economic model predictive control, nonlinear model identification, regression, process control

## 1. INTRODUCTION

System identification (Ljung, 1999) has been an important technique in the process industries for obtaining linear process models for use in tracking model predictive control (MPC) (Qin and Badgwell, 2003). The development of EMPC (Ellis et al., 2014; Rawlings et al., 2012; Müller and Allgöwer, 2017), in which the objective function of the MPC can be non-quadratic and economics-based, raises questions on the continued effectiveness of traditional empirical models in EMPC such as: 1) how to prevent the profit from being potentially highly restricted by the accuracy of linear empirical models in possibly only a relatively small neighborhood of the steady-state (Alanqar et al., 2015b); 2) how to develop a profit-based objective function for a process for which the dynamics are not understood (i.e., the freedom introduced into MPC by not requiring a pre-specified quadratic objective function form may also necessitate a greater understanding of the process physics so that an appropriate objective function form can be selected); and 3) how to ensure that appropriate constraints can be developed on physical quantities, given that an EMPC does not necessarily confine the closed-loop state to a neighborhood of the origin and therefore state constraints can be critical from a safety standpoint.

Motivated by the above considerations, we seek to develop a methodology for on-line EMPC development that focuses on obtaining a more physically-meaningful model than can be provided with traditional system identification techniques for use in developing the required objective function, constraints, and model of the EMPC from on-line operating data. Specifically, an EMPC design is developed with terms in the objective function and constraints that can be turned on or off for short periods of time to facilitate the collection of non-routine (and ideally, very specific and targeted) operating data which can be used for better understanding the underlying physics of the process to aid in the development of appropriate process models with which to update the EMPC design. The flexibility of the proposed approach derived from the generality of EMPC (e.g., the ability to utilize any objective function and constraints and to enforce time-varying operating policies that maintain closed-loop stability) is intended to be utilized to develop input policies for model identification that are distinct from policies which seek to excite the process dynamics on-line to identify the parameters of an assumed model or aid in state estimation with an assumed model (Heirung et al., 2015; Marafioti et al., 2014; Houska et al., 2017; Larsson et al., 2013). Specifically, the proposed strategy ideally can be utilized to seek to force the data generated under the input policies to have certain structures (e.g., by forcing the data to be obtained from a case where one variable is at an approximately fixed value while another is varied) that may be conducive to better understanding relationships between variables and measured quantities in the process model and for therefore

⋆ Financial support from Wayne State University is gratefully acknowledged.

proposing and verifying mathematical forms for the terms in the model that are consistent with the resulting data.

## 2. PRELIMINARIES

### 2.1 Notation

The Euclidean norm of a vector is denoted by $|\cdot|$. The function $\alpha(\cdot) : [0, a) \to [0, \infty)$ belongs to class $\mathcal{K}$ if it is strictly increasing and $\alpha(0) = 0$. We define $\Omega_\rho := \{x \in \mathbb{R}^n : V(x) \leq \rho\}$ where $V$ is a sufficiently smooth, positive definite function and the symbol $S(\Delta)$ denotes the family of piecewise constant functions with period $\Delta$. Set subtraction is signified by / (i.e., $x \in A/B := \{x \in A : x \notin B\}$). The notation diag$(x)$ with $x \in \mathbb{R}^n$ represents an $n \times n$ matrix with the entries of the vector $x$ on its diagonal. The transpose of the vector $x$ is denoted by $x^T$.

### 2.2 Class of Systems

The class of nonlinear systems considered is:

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

where $f$ is a nonlinear locally Lipschitz vector function of the state vector of the system $x \in X \subset \mathbb{R}^n$, the manipulated input vector $u \in \mathbb{R}^m$ and the disturbance vector $w \in \mathbb{R}^l$, where $X$ represents the state constraint set. The inputs are constrained in $U := \{u \in \mathbb{R}^m : {u_i}^{min} \leq u_i \leq {u_i}^{max}, i = 1, ..., m\}$, while $w \in W := \{w \in \mathbb{R}^l : |w(t)| \leq \Theta, \Theta > 0\}$, $W \subset \mathbb{R}^l$. We will refer to Eq. 1 as the nominal system when $w(t) \equiv 0$. We consider $f(0, 0, 0) = 0$. The state is measured at each sampling time $t_k = k\Delta$ where $k = 0, 1, \ldots,$ and $\Delta$ is the sampling period. We consider stabilizable nonlinear systems (i.e., there exists an explicit stabilizing Lyapunov-based controller $h(x)$ that is locally Lipschitz and renders the origin asymptotically stable in the sense that there exists a sufficiently smooth Lyapunov function $V : \mathbb{R}^n \to \mathbb{R}_+$ such that:

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

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

$$h(x) \in U \tag{2c}$$

for all $x \in D \subset \mathbb{R}^n$, where $D$ is an open neighborhood of the origin and the $\alpha_i(\cdot)$, $i = 1, 2, 3, 4$, are functions of class $\mathcal{K}$). We define $\Omega_\rho \subset D$ to be the stability region of the nominal closed-loop system under the controller $h(x)$ and require that it be chosen such that $x \in X$, $\forall x \in \Omega_\rho$. The following inequality holds:

$$\begin{aligned} &\left|\frac{\partial V(x_1)}{\partial x} f(x_1, u, w) - \frac{\partial V(x_2)}{\partial x} f(x_2, u, 0)\right| \\ &\qquad \leq L'_x|x_1 - x_2| + L'_w|w| \end{aligned} \tag{3}$$

$\forall x_1, x_2 \in \Omega_\rho$, $u \in U$ and $w \in W$, where $L'_x > 0$ and $L'_w > 0$. Moreover, there exists $M > 0$ such that:

$$|f(x, u, w)| \leq M \tag{4}$$

$\forall x \in \Omega_\rho$, $u \in U$, and $w \in W$ for bounded $M$.

We assume that only an empirical model is available:

$$\dot{\hat{x}}(t) = f_{NL}(\hat{x}(t), u(t)) \tag{5}$$

where $f_{NL}$ is assumed to be a locally Lipschitz nonlinear vector function with $f_{NL}(0, 0) = 0$. We consider empirical models for which the origin can be rendered asymptotically stable by a locally Lipschitz explicit stabilizing controller $h_{NL}(x)$ in the sense that:

$$\hat{\alpha}_1(|x|) \leq \hat{V}(x) \leq \hat{\alpha}_2(|x|) \tag{6a}$$

$$\frac{\partial \hat{V}(x)}{\partial x} f_{NL}(x, h_{NL}(x)) \leq -\hat{\alpha}_3(|x|) \tag{6b}$$

$$\left|\frac{\partial \hat{V}(x)}{\partial x}\right| \leq \hat{\alpha}_4(|x|) \tag{6c}$$

$$h_{NL}(x) \in U \tag{6d}$$

for all $x \in D_{NL}$, where $\hat{V} : \mathbb{R}^n \to \mathbb{R}_+$ is a sufficiently smooth Lyapunov function and $\hat{\alpha}_i, i = 1, 2, 3, 4$, are class $\mathcal{K}$ functions. We define $\Omega_{\hat{\rho}} \subset D_{NL}$ as the stability region of the system of Eq. 5 and require that $x \in X$, $\forall x \in \Omega_{\hat{\rho}}$. There exist $M_L > 0$ and $L_L > 0$ such that:

$$|f_{NL}(x, u)| \leq M_L \tag{7a}$$

$$\begin{aligned} &\left|\frac{\partial \hat{V}(x_1)}{\partial x} f_{NL}(x_1, u) - \frac{\partial \hat{V}(x_2)}{\partial x} f_{NL}(x_2, u)\right| \\ &\qquad \leq L_L|x_1 - x_2| \end{aligned} \tag{7b}$$

$\forall x, x_1, x_2 \in \Omega_{\hat{\rho}}$ and $u \in U$. Furthermore:

$$|f(x_1, u, w) - f(x_2, u, 0)| \leq \bar{L}_x|x_1 - x_2| + \bar{L}_w|w| \tag{8a}$$

$$\begin{aligned} &\left|\frac{\partial \hat{V}(x_1)}{\partial x} f(x_1, u, w) - \frac{\partial \hat{V}(x_2)}{\partial x} f(x_2, u, 0)\right| \\ &\qquad \leq \bar{L}'_x|x_1 - x_2| + \bar{L}'_w|w| \end{aligned} \tag{8b}$$

$\forall x_1, x_2 \in \Omega_{\hat{\rho}}$, $u \in U$, and $w \in W$, and $\bar{L}_x$, $\bar{L}_w$, $\bar{L}'_x$, and $\bar{L}'_w$ as positive constants.

## 3. DATA-GATHERING LYAPUNOV-BASED EMPC FORMULATION

In this section, we present the concept that an EMPC may be able to operate the process of Eq. 1 in a non-routine fashion for short periods of time to seek to obtain data for developing and validating physics-based empirical models. It seeks to do this through the addition of terms in the objective function or activation conditions for the constraints that can be turned on for short periods of time. An example of such a data-gathering EMPC is:

$$\begin{aligned} \min_{u(t) \in S(\Delta)} \int_{t_k}^{t_{k+N}} &[L_e(\hat{x}(\tau), u(\tau)) + \delta_1 \sum_{j=1}^{n_k} \alpha_{wj}(u_j(\tau) - u_{d,j})^2 \\ &+ \delta_2 \sum_{i=1}^{n_s} \alpha_{yi}(\hat{x}_i(\tau) - x_{d,i})^2] d\tau \end{aligned} \tag{9a}$$

$$\text{s.t.} \quad \dot{\hat{x}} = f_{NL}(\hat{x}(t), u(t)) \tag{9b}$$

$$\hat{x}(t_k) = x(t_k) \tag{9c}$$

$$\hat{x}(t) \in X,\ \forall\, t \in [t_k, t_{k+N}) \tag{9d}$$

$$u(t) \in U,\ \forall\, t \in [t_k, t_{k+N}) \tag{9e}$$

$$\hat{V}(\hat{x}(t)) \leq \hat{\rho}_e,\ \ \forall\, t \in [t_k, t_{k+N}) \ \text{ if } \ x(t_k) \in \Omega_{\hat{\rho}_e} \tag{9f}$$

$$\begin{aligned} &\frac{\partial \hat{V}(x(t_k))}{\partial x}(f_{NL}(x(t_k), u(t_k))) \\ &\qquad \leq \frac{\partial \hat{V}(x(t_k))}{\partial x} (f_{NL}(x(t_k), h_{NL}(x(t_k)))), \\ &\qquad \text{if } \ x(t_k) \notin \Omega_{\hat{\rho}_e} \ \text{ or } \ \delta_3 = 1 \end{aligned} \tag{9g}$$

where $u(t) \in S(\Delta)$ signifies that the optimization variable of Eq. 9 is a piecewise-constant vector function with period

$\Delta$. This formulation is a form of Lyapunov-based EMPC (LEMPC) (Heidarinejad et al., 2012) using an empirical process model (Alanqar et al., 2015b,a). $L_e$ (Eq. 9a) is a measure of the process economics to be minimized during routine operation (i.e., when $\delta_1 = \delta_2 = \delta_3 = 0$). The empirical model of Eq. 9b with the initial condition in Eq. 9c obtained from a measurement of the process state at $t_k$ is used in evaluating whether the inputs computed by the LEMPC will optimize the objective function of Eq. 9 and whether they will cause the state constraints in Eq. 9d to be met. The input trajectories returned by the LEMPC must furthermore meet the input constraint in Eq. 9e.

$\delta_1$, $\delta_2$, and $\delta_3$, are parameters in Eq. 9 that take a value of either zero or one, which allows them to be used to either enforce routine operation (when they all take values of zero) or non-routine operation (when one or more of them takes a value of 1 at a given sampling time). They do not depend on the process state or inputs, and therefore can be turned on (set to 1) for arbitrarily long or short periods of time to facilitate a type of on-line experimentation focused on gathering data that aids in better understanding the physics of a process or validating an empirical model with specific data expected to verify whether certain terms of the model have been correctly developed. For example, when $\delta_1 = 1$, the first $n_k$ input vector components $u_j$ may be driven toward desired values $u_{d,j}$ if the penalty term $\alpha_{wj}$ is appropriately selected since setting $\delta_1$ to 1 activates the soft constraint on $u_j$, $j = 1, \ldots, n_k$, in the objective function of Eq. 9. Similarly, when $\delta_2 = 1$, a soft constraint is imposed on the difference between the predictions $\hat{x}_i$ of the first $n_s$ components of the state vector and their desired values $x_{d,i}$, weighted in the objective function with penalty $\alpha_{yi}$. The constraint of Eq. 9f requires the LEMPC to maintain the predictions of the closed-loop state obtained from the empirical model of Eq. 9b in the level set $\Omega_{\hat{\rho}_e} \subset \Omega_{\hat{\rho}}$ of $\hat{V}$. The constraint of Eq. 9g drives the closed-loop state to level sets of $\hat{V}$ with a lower upper bound. Though the constraints of Eqs. 9f-9g are activated under routine operation by the location of $x(t_k)$ in state-space, when $\delta_3 = 1$, Eq. 9g is activated repeatedly regardless of whether $x(t_k) \in \Omega_{\hat{\rho}_e}$ or not. If $\delta_3 = 1$ for a sufficient number of subsequent sampling periods, the closed-loop state is driven to a neighborhood of the origin under sufficient conditions such as a sufficiently small $\Delta$ and $\Theta$. After the LEMPC of Eq. 9 is used to obtain non-routine process data that may help with developing and validating more physically-based process models, then $f_{NL}$, $\hat{\rho}$, $\hat{\rho}_e$, $\hat{V}$, and $h_{NL}$ in Eq. 9 can be updated.

## 4. DATA-GATHERING LEMPC STABILITY ANALYSIS

In this section, we prove recursive feasibility and closed-loop stability of the process of Eq. 1 under the LEMPC of Eq. 9. We begin with three propositions and then introduce the main results that use them in a theorem.

*Proposition 1.* (Alanqar et al., 2015a) Consider the systems

$$\dot{x}_a = f(x_a(t), u(t), w(t)) \tag{10a}$$

$$\dot{x}_b = f_{NL}(x_b(t), u(t)) \tag{10b}$$

with initial states $x_a(t_0) = x_b(t_0) \in \Omega_{\hat{\rho}}$ with $t_0 = 0$, $u \in U$, and $w \in W$. If $x_a(t), x_b(t) \in \Omega_{\hat{\rho}}$ for $t \in [0, T]$ then there exists a function $f_W(\cdot)$ such that:

$$|x_a(t) - x_b(t)| \leq f_W(t) \tag{11}$$

with:

$$f_W(t) := \frac{\bar{L}_w \Theta + M_{err}}{\bar{L}_x}(e^{\bar{L}_x t} - 1) \tag{12}$$

where $M_{err}$ is defined by:

$$|f(x, u, 0) - f_{NL}(x, u)| \leq M_{err} \tag{13}$$

$\forall x \in \Omega_{\hat{\rho}}$ and $u \in U$.

*Proposition 2.* (Mhaskar et al., 2013) Consider the Lyapunov function $\hat{V}(\cdot)$ of the nominal system of Eq. 5 under the controller $h_{NL}(x)$ that meets Eq. 6. There exists a quadratic function $f_V(\cdot)$ such that:

$$\hat{V}(x) \leq \hat{V}(\bar{x}) + f_V(|x - \bar{x}|) \tag{14}$$

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

$$f_V(s) = \hat{\alpha}_4(\hat{\alpha}_1^{-1}(\hat{\rho}))s + M_v s^2 \tag{15}$$

where $M_v$ is a positive constant.

*Proposition 3.* (Muñoz de la Peña and Christofides, 2008) Consider the closed-loop system of Eq. 5 under $h_{NL}(\hat{x})$ that satisfies the inequalities of Eq. 6 in sample-and-hold. Let $\Delta > 0$, $\hat{\epsilon}_W > 0$, and $\hat{\rho} > \hat{\rho}_e > \hat{\rho}_{\min} > \hat{\rho}_s > 0$ satisfy:

$$-\hat{\alpha}_3(\hat{\alpha}_2^{-1}(\hat{\rho}_s)) + L_L M_L \Delta \leq -\hat{\epsilon}_W/\Delta \tag{16}$$

and

$$\hat{\rho}_{\min} := \max\{\hat{V}(\hat{x}(t + \Delta)) \quad : \quad \hat{V}(\hat{x}(t)) \leq \hat{\rho}_s\}. \tag{17}$$

If $\hat{x}(0) \in \Omega_{\hat{\rho}}$, then:

$$\hat{V}(\hat{x}(t_{k+1})) - \hat{V}(\hat{x}(t_k)) \leq -\hat{\epsilon}_W \tag{18}$$

for $\hat{x}(t_k) \in \Omega_{\hat{\rho}}/\Omega_{\hat{\rho}_s}$ and the state trajectory $\hat{x}(t)$ of the closed-loop system is always bounded in $\Omega_{\hat{\rho}}$ for $t \geq 0$ and is ultimately bounded in $\Omega_{\hat{\rho}_{\min}}$.

*Theorem 4.* Consider the closed-loop system of Eq. 1 under the LEMPC of Eq. 9 based on the controller $h_{NL}(x)$ that satisfies the inequalities in Eq. 6. Let $\epsilon_W > 0$, $\Delta > 0$, $N \geq 1$, and $\hat{\rho} > \hat{\rho}_e > \hat{\rho}_{\min} > \hat{\rho}_s > 0$ satisfy:

$$\begin{aligned} &- \hat{\alpha}_3(\hat{\alpha}_2^{-1}(\hat{\rho}_e)) + \hat{\alpha}_4(\hat{\alpha}_1^{-1}(\hat{\rho}))M_{err} + \bar{L}'_x M \Delta \\ &\quad + \bar{L}'_w \Theta \leq -\epsilon_W/\Delta \end{aligned} \tag{19}$$

$$\hat{\rho}_e \leq \hat{\rho} - f_V(f_W(\Delta)) \tag{20}$$

If $x(0) \in \Omega_{\hat{\rho}}$, and Proposition 3 is satisfied, then the state trajectory $x(t)$ of the closed-loop system is always bounded in $\Omega_{\hat{\rho}}$ for $t \geq 0$.

**Proof.** From Proposition 3 and Eq. 6d, Eqs. 9d, 9e, and 9f are met under $h_{NL}$ in sample-and-hold because that control law maintains the closed-loop state in $\Omega_{\hat{\rho}_e}$ when $x(t_k) \in \Omega_{\hat{\rho}_e}$ for $\hat{\rho}_e > \hat{\rho}_{\min}$ and then it maintains the closed-loop state in $\Omega_{\hat{\rho}_{\min}}$. Eq. 9g is trivially satisfied by $h_{NL}(\hat{x}(t_k))$. Feasibility of each constraint of Eq. 9 is thus established at every sampling time for any $\delta_i$, $i = 1, 2, 3$. Therefore, we now prove that if $x(t_0) \in \Omega_{\hat{\rho}}$, $x(t) \in \Omega_{\hat{\rho}}$, $\forall t \geq 0$. If $x(t_k) \in \Omega_{\hat{\rho}}/\Omega_{\hat{\rho}_e}$, then from Eqs. 9g and 6b:

$$\begin{aligned} &\frac{\partial \hat{V}(x(t_k))}{\partial x}(f_{NL}(x(t_k), u(t_k))) \\ &\leq \frac{\partial \hat{V}(x(t_k))}{\partial x}(f_{NL}(x(t_k), h_{NL}(x(t_k)))) \leq -\hat{\alpha}_3(|x(t_k)|) \end{aligned} \tag{21}$$

A bound on $\frac{\partial \hat{V}(x(t_k))}{\partial x}(f(x(t_k), h_{NL}(x(t_k)), 0))$ can also be developed by adding and subtracting $\frac{\partial \hat{V}(x(t_k))}{\partial x}(f_{NL}(x(t_k), h_{NL}(x(t_k))))$ from it giving:

$$\frac{\partial \hat{V}(x(t_k))}{\partial x}\,(f(x(t_k), h_{NL}(x(t_k)), 0)) \le -\hat{\alpha}_3(|x(t_k)|) + \hat{\alpha}_4(|x(t_k)|)M_{err} \tag{22}$$

for any $x(t_k) \in \Omega_{\hat{\rho}}$, which follows from Eqs. 13 and 6c. $\frac{\partial \hat{V}(x(\tau))}{\partial x}\,(f(x(\tau), h_{NL}(x(t_k)), w(\tau)))$ for $\tau \in [t_k, t_{k+1})$ is:

$$\frac{\partial \hat{V}(x(\tau))}{\partial x}\,(f(x(\tau), h_{NL}(x(t_k)), w(\tau))) \tag{23a}$$

$$\le \bar{L}'_x M\Delta + \bar{L}'_w \Theta - \hat{\alpha}_3(\hat{\alpha}_2^{-1}(\hat{\rho}_e)) + \hat{\alpha}_4(\hat{\alpha}_1^{-1}(\hat{\rho}))M_{err} \tag{23b}$$

for $\tau \in [t_k, t_{k+1})$, which follows from Eqs. 22, 8b, and 6, the bound on $w$, Eq. 4, and the continuity of $x$. Following similar steps as in Eq. 22 but adding and subtracting $\frac{\partial \hat{V}(x(t_k))}{\partial x}\,(f_{NL}(x(t_k), u(t_k)))$ and using Eq. 21, we obtain:

$$\frac{\partial \hat{V}(x(t_k))}{\partial x}\,(f(x(t_k), u(t_k), 0)) \le -\hat{\alpha}_3(|x(t_k)|) + \hat{\alpha}_4(|x(t_k)|)M_{err} \tag{24}$$

Eq. 24 can be used in the following with similar steps as were taken to arrive at Eq. 23b:

$$\frac{\partial \hat{V}(x(\tau))}{\partial x}\,(f(x(\tau), u(t_k), w(\tau))) \le -\hat{\alpha}_3(\hat{\alpha}_2^{-1}(\hat{\rho}_e)) + \hat{\alpha}_4(\hat{\alpha}_1^{-1}(\hat{\rho}))M_{err} + \bar{L}'_x M\Delta + \bar{L}'_w \Theta \tag{25}$$

for $\tau \in [t_k, t_{k+1})$. From Eqs. 25 and 19:

$$\begin{aligned} &\hat{V}(x(t_{k+1})) - \hat{V}(x(t_k)) \le -\epsilon_W \\ &\hat{V}(x(\tau)) \le \hat{V}(x(t_k)), \quad \forall \tau \in [t_k, t_{k+1}] \end{aligned} \tag{26}$$

when $x(t_k) \in \Omega_{\hat{\rho}}/\Omega_{\hat{\rho}_e}$, and the Lyapunov function value will decrease over a sampling period, and $x(t) \in \Omega_{\hat{\rho}}$, $\forall t \in [t_k, t_{k+1}]$. This indicates that if the constraint of Eq. 9g is applied for consecutive sampling periods, then in a finite number of sampling periods, $x(t)$ will re-enter the region $\Omega_{\hat{\rho}_e}$. When $x(t_k) \in \Omega_{\hat{\rho}_e}$, the following holds from Propositions 1-2 and Eq. 9f if $x(t) \in \Omega_{\hat{\rho}}$ for $t \in [t_k, t_{k+1})$:

$$\hat{V}(x(t)) \le \hat{\rho}_e + f_V(f_W(\Delta)) \tag{27}$$

for $t \in [t_k, t_{k+1})$. If Eq. 20 holds, $\hat{V}(x(t)) \le \hat{\rho}$ for $t \in [t_k, t_{k+1})$ and therefore when $x(t_k) \in \Omega_{\hat{\rho}_e}$, $x(t) \in \Omega_{\hat{\rho}}$ for $t \in [t_k, t_{k+1})$ as assumed. Because $x(t) \in \Omega_{\hat{\rho}}$ for $t \in [t_k, t_{k+1})$ if $x(t_k) \in \Omega_{\hat{\rho}}/\Omega_{\hat{\rho}_e}$ or $x(t_k) \in \Omega_{\hat{\rho}_e}$, $x(t) \in \Omega_{\hat{\rho}}$ for all $t \ge 0$ if $x(t_0) \in \Omega_{\hat{\rho}}$. This proof was independent of the value of $\delta_i$, $i = 1, 2, 3$. This completes the proof.

*Remark 5.* An important goal of the assumptions in Section 2.2 and of the results of the proof above is that they allow characterization of conditions under which the proposed EMPC can maintain closed-loop stability of a nonlinear process. This is important for understanding relationships among tuning parameters of the control design (e.g., various parameters in Eq. 19 such as $\Delta$ must be sufficiently small to guarantee closed-loop stability). This provides intuition on which parameters to adjust and how to adjust them when designing a controller of the proposed type even if all equations used in developing the theory (e.g., $h(x)$ and $\hat{\alpha}_i$, $i = 1, \ldots, 3$) are not known.

## 5. APPLICATION TO A CHEMICAL PROCESS EXAMPLE

To demonstrate the use of an EMPC with data-gathering functionality, we consider an illustrative continuous stirred tank reactor (CSTR) example where the reaction $A \rightarrow B$ occurs. The feed to the reactor (with volumetric flow rate $F$) contains $A$ in an inert solvent at concentration $C_{A0}$ and temperature $T_0$. A jacket is used to heat/cool the reactor at rate $Q$. The liquid density ($\rho_L$), heat capacity $C_p$ and liquid volume $V$ are constants with the values in (Alanqar et al., 2015b). The process dynamics are given as follows:

$$\frac{dC_A}{dt} = \frac{F}{V}(C_{A0} - C_A) - k_0 e^{-\frac{E}{R_g T}} C_A^2 \tag{28a}$$

$$\frac{dT}{dt} = \frac{F}{V}(T_0 - T) - \frac{\Delta H k_0}{\rho_L C_p} e^{-\frac{E}{R_g T}} C_A^2 + \frac{Q}{\rho_L C_p V} \tag{28b}$$

where $C_A$ is the concentration of $A$ and $T$ is the temperature of the reactor. The reaction inside the CSTR has pre-exponential factor $k_0$, enthalpy of reaction $\Delta H$, and activation energy $E$. $R_g$ is the ideal gas constant. The manipulated inputs $C_{A0}$ and $Q$ are constrained: $0.5 \le C_{A0} \le 7.5$ $\frac{kmol}{m^3}$ and $-5 \times 10^5 \le Q \le 5 \times 10^5$ $\frac{kJ}{hr}$. The process is operated around the steady-state $C_{As} = 1.22$ $\frac{kmol}{m^3}$, $T_s = 438.2$ $K$, $C_{A0s} = 4$ $\frac{kmol}{m^3}$, and $Q_s = 0$ $\frac{kJ}{hr}$. We define the following deviation variable vectors: $x = [x_1\ x_2]^T = [C_A - C_{As}\ T - T_s]^T$ and $u = [u_1\ u_2]^T = [C_{A0} - C_{A0s}\ Q - Q_s]^T$.

The control objective is to operate the system of Eq. 28 in a manner that maximizes the production rate of the desired product, respects the input constraints, and maintains closed-loop stability. However, we assume that the reaction rate law in Eq. 28 is unknown; therefore, it is not possible to design an LEMPC that maximizes the production rate because the equation for the production rate is not known. We assume that we know that the process model has the form in Eq. 28, but we do not know the form of the reaction rate expression and therefore do not have the first-principles model available. Instead, the following linear empirical model from (Alanqar et al., 2015b) is available:

$$\dot{\hat{x}}_1 = -34.5\hat{x}_1 - 0.473\hat{x}_2 + 5.24u_1 - 8.09 \times 10^{-6}u_2 \tag{29a}$$

$$\dot{\hat{x}}_2 = 1430\hat{x}_1 + 18.1\hat{x}_2 - 11.6u_1 + 4.57 \times 10^{-3}u_2 \tag{29b}$$

This model is used to design constraints for an LEMPC with $\hat{V} = x^T P x$ (alternative Lyapunov functions could also be explored in the proposed context), where $P = [1060\ 22; 22\ 0.52]$. The Lyapunov-based controller from (Alanqar et al., 2015b) is used, which sets $h_{NL}(x) = [h_{NL,1}(x)\ h_{NL,2}(x)]^T = [0\ h_{NL,2}(x)]^T$, where $h_{NL,2}(x)$ is determined from Sontag's control law (Sontag, 1989) applied to the system of Eq. 29 and $\hat{\rho} = 64.3$ and $\hat{\rho}_e = 55$.

Due to the unavailability of a production rate model for designing $L_e$, we initially utilize a quadratic stage cost:

$$L_e = \hat{x}^T Q \hat{x} + u^T R u \tag{30}$$

where $Q = \text{diag}(10^4, 100)$ and $R = \text{diag}(10^4, 10^{-6})$. The constraint of Eq. 9f is imposed at the end of each sampling period. When Eq. 9g is activated at $t_k$, we impose Eq. 9f at the end of sampling periods 2 to $N$.

We would like to modify the objective function of Eq. 30 for short periods of time to seek to obtain non-routine operating data that may aid in obtaining a more physically-based process model. To do this, we introduce the concept of an operating period with length $t_p = 1$ $hr$ for use in characterizing the time periods over which the objective function modifications are used, and operate the process under LEMPC but with the stage cost of Eq. 30 replaced for certain time periods with the following stage costs:

$$L_e = \hat{x}^T Q \hat{x} + u^T R u + 10^4(10000(\hat{x}_1 - x_{1,fix})^2 - 10000(u_1 - u_1^*(t_{k-1}))^2 + (u_2 - u_2^*(t_{k-1}))^2) \quad (31a)$$

$$L_e = \hat{x}^T Q \hat{x} + u^T R u + 10^4(10^{10}(\hat{x}_1 - x_{1,fix})^2 - 10000(u_1 - u_1^*(t_{k-1}))^2 + 10^{-6}(u_2 - u_2^*(t_{k-1}))^2) \quad (31b)$$

$$L_e = 10^4(100(\hat{x}_2 - x_{2,fix})^2) \quad (31c)$$

$$L_e = 10^4(100(\hat{x}_2 - x_{2,fix})^2 + c_T(\hat{x}_1 - x_{1,fix})^2) \quad (31d)$$

where $c_T$ is a constant. The stage cost of Eq. 31a was used at the 20th, 21st, and 22nd sampling periods in the operating period between $t = 15\ hr$ and $t = 16\ hr$ with $x_{1,fix} = 0.2$ ($u_1^*(t_{k-1})$ and $u_2^*(t_{k-1})$ represent the values of $u_1$ and $u_2$ implemented at the prior sampling time), and at the 50th, 51st, and 52nd sampling periods in the operating period with $x_{1,fix} = 0.4$. At the 60th, 61st, and 62nd sampling periods in the operating period between $t = 15\ hr$ and $t = 16\ hr$, Eq. 31b was used with $x_{1,fix} = 0$. At the 90th, 91st, and 92nd sampling periods in the operating period between $t = 15\ hr$ and $t = 16\ hr$, Eq. 31a with $x_{1,fix} = 0.2$ was used. For the 18th operating period, Eq. 31c was used with $x_{2,fix} = 2.203$. In the 19th, 20th, 21st, 22nd, 23rd, 24th, and 25th operating periods, Eq. 31d was used with $x_{2,fix} = 2.203$ and $x_{1,fix}$ varying so that in the seven operating periods, it was set to 0.15, 0.14, 0.13, 0.12, 0.11, 0.12, and 0.12, respectively. For the 27th, 28th, 29th, 30th, 31st, 32nd, 33rd, and 34th operating periods, Eq. 31d was used with $x_{2,fix} = 2.203$, 4, 5, 2, 1, 0, $-1$, and $-2$, respectively, and $x_{1,fix} = 0.12$. $c_T$ was set to 1000 in Eq. 31d in the 19th-25th and 27th operating periods, and to 10000 in the 28th-34th operating periods. In the simulations, $N = 10$ and $\Delta = 0.01\ hr$. The empirical model of Eq. 29 was integrated within the EMPC with an integration step of $10^{-4}\ hr$, and the first-principles model of Eqs. 28a-28b representing the process was numerically integrated with the same integration step. The input $h_{NL}$ was not saturated at its bounds in the LEMPC or set to zero at the steady-state. The simulations were performed utilizing the interior point solver of the MATLAB function fmincon in MATLAB R2016a by MathWorks®. Exit flags indicating that a local minimum was found or that it was possible were accepted. The simulations were initialized from $x_1 = -0.4\ \frac{kmol}{m^3}$ and $x_2 = 20\ K$.

The series of stage costs in Eq. 31 allowed $T$ to be approximately constant while $C_A$ varied from the 19th to the 25th operating periods, and allowed $C_A$ to be approximately constant while $T$ was varied from the 27th to 34th operating periods. This means that if the reaction rate at various times in these operating periods can be obtained, the acquired data is in a form suitable for examining how the temperature and concentration affect the reaction rate individually (and thus for proposing a form of the reaction rate law; for this example, this type of structure to the data was determined to be desirable for identifying the mathematical form of the rate law and therefore was targeted using Eqs. 31a-31d). To obtain the reaction rate at various times in the operating periods, we utilized the state and input measurements assumed to be available every $10^{-4}\ hr$, and a backward finite difference approximation of $\dot{C}_A$ and $\dot{T}$ with the measured values of $C_A$ and $T$, to determine the reaction rates at various times from a linear regression on the obtained data in the spirit of the work in (Brunton et al., 2016) by setting up the following matrices:

$$\begin{bmatrix} \ln(-(\dot{C}_A(\tilde{t}_1) - \frac{F}{V}(C_{A0}(\tilde{t}_1) - C_A(\tilde{t}_1)))) \\ \ln(\dot{T}(\tilde{t}_1) - \frac{F}{V}(T_0 - T(\tilde{t}_1)) - \frac{Q(\tilde{t}_1)}{\rho_L c_p V}) \\ \vdots \\ \ln(-(\dot{C}_A(\tilde{t}_q) - \frac{F}{V}(C_{A0}(\tilde{t}_q) - C_A(\tilde{t}_q)))) \\ \ln(\dot{T}(\tilde{t}_q) - \frac{F}{V}(T_0 - T(\tilde{t}_q)) - \frac{Q(\tilde{t}_q)}{\rho_L c_p V}) \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 1 & 1 & 0 & \cdots & 0 \\ & & \vdots & & \\ 0 & 0 & 0 & \cdots & 1 \\ 1 & 0 & 0 & \cdots & 1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \\ c_{q+1} \end{bmatrix} \quad (32)$$

where the $\tilde{t}_i$, $i = 1, \ldots, q$, represent the times corresponding to the measurements of $C_A$, $T$, $Q$, and $C_{A0}$ which are utilized in Eq. 32 ($\tilde{t}_1$ represents the first time utilized). $c_1$ corresponds to $\ln(\frac{-\Delta H}{\rho_L C_p})$, and $c_2, \ldots, c_{q+1}$ correspond to the logarithms of the reaction rates associated with each time $\tilde{t}_i$, $i = 1, \ldots, q$ (where these reaction rates will be denoted by $r_1(\tilde{t}_i)$). $q$ was set to 400 in Eq. 32. Fifty values of the states, inputs, and derivatives of the states were utilized from approximately halfway through each of the 8 operating periods between the 18th and 25th for obtaining the $C_A$ dependence of $r_1$, and fifty values of the states, inputs, and derivatives of the states were utilized from approximately halfway through each of the 8 operating periods between the 27th and 34th for obtaining the $T$ dependence of $r_1$. Scatter plots of the variations of the regressed values of the reaction rates with temperature and concentration gave a relatively linear relationship between $\ln(r_1)$ against $\ln(C_A)$ when $T$ was fixed and a relatively linear plot of $\ln(r_1)$ versus $1/T$ when $C_A$ was fixed, leading to the postulate that a reasonable form of the rate law would be $k_0 e^{-E/(R_g T)} C_A^d$, with $d$ a parameter to be fit.

With the postulated rate law form, a regression similar to that in Eq. 32 can be performed but with the matrix and vector on the right-hand side as follows:

$$\begin{bmatrix} 1 & \frac{1}{T(\tilde{t}_1)} & \ln(C_A(\tilde{t}_1)) & 0 \\ 1 & \frac{1}{T(\tilde{t}_1)} & \ln(C_A(\tilde{t}_1)) & 1 \\ & & \vdots & \\ 1 & \frac{1}{T(\tilde{t}_q)} & \ln(C_A(\tilde{t}_q)) & 0 \\ 1 & \frac{1}{T(\tilde{t}_q)} & \ln(C_A(\tilde{t}_q)) & 1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix} \quad (33)$$

$c_1$, $c_2$, $c_3$, and $c_4$ correspond to $\ln(k_0)$, $\frac{-E}{R_g}$, $d$, and $\ln(\frac{-\Delta H}{\rho_L C_p})$, respectively. Data from the first 9501 integration steps was utilized for the regression (i.e., $q = 9500$ since $\dot{C}_A$ and $\dot{T}$ are not considered at $t_0$). The results ($k_0 = 8977447.8\ \frac{m^3}{hr\ kmol}$, $\Delta H = -11498.19\ \frac{kJ}{kmol}$, $E = 50223.73\ \frac{kJ}{kmol}$, and $d = 2.01$) are close to the actual values.

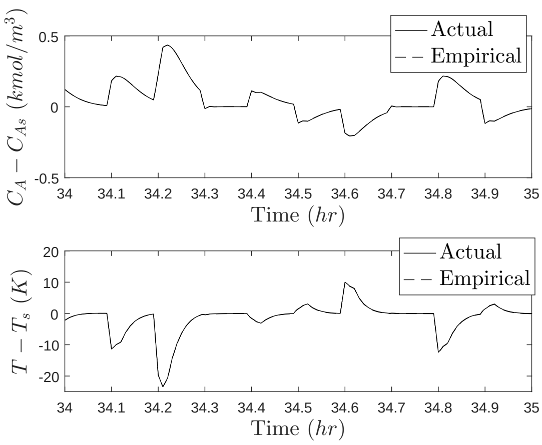


Fig. 1. Profiles for $x_1$ (top plot) and $x_2$ (bottom plot) from the process and predicted by the empirical model of Eq. 33 in the 35th operating period (the empirical model results almost overlay the process data).

To validate this model, we utilized the data generated until this point as well as additional data generated by the controller by augmenting the stage cost of Eq. 30 with the following terms in the 35th operating period:

$$10^8(\hat{x}_1 - x_{1,fix})^2 - 10^2(u_1 - u_1^*(t_{k-1}))^2 - 10^{-8}(u_2 - u_2^*(t_{k-1}))^2 \tag{34}$$

where $x_{1,fix} = 0.2$ for the 10th, 11th, and 12th sampling times of the 35th operating period, $x_{1,fix} = 0.4$ for the 20th, 21st, and 22nd sampling times, $x_{1,fix} = 0$ for the 30th, 31st, and 32nd sampling times, $x_{1,fix} = 0.1$ for the 40th, 41st, and 42nd sampling times, $x_{1,fix} = -0.1$ for the 50th, 51st, and 52nd sampling times, $x_{1,fix} = -0.2$ for the 60th, 61st, and 62nd sampling times, $x_{1,fix} = 0$ for the 70th, 71st, and 72nd sampling times, $x_{1,fix} = 0.2$ for the 80th, 81st, and 82nd sampling times, and $x_{1,fix} = -0.1$ for the 90th, 91st, and 92nd sampling times. Fig. 1 shows the relatively good agreement between the measured data and the results generated by the identified empirical model of Eq. 33 initiated from $x_{init}$ with the same inputs as were applied to the system of Eq. 28 throughout the 35 operating periods, with a close-up of the results from the last operating period to indicate the agreement with the variations in the stage cost according to Eq. 34. This indicates the potential of an LEMPC with the ability to operate a process in a non-routine fashion for some period of time to aid in obtaining data that is expected to allow properties of the underlying physics to be ascertained or to allow models to be verified using data different from that used in building the model, before updating an LEMPC to reflect the new model. The identified model for the example includes a term for the production rate of the desired product $(k_0 e^{-E/(R_g T)} C_A^d)$ which can be used to redesign the EMPC with a profit-based objective function.

## 6. CONCLUSION

A data-gathering EMPC design has been developed that activates hard and soft constraints for short periods of time to seek to obtain data from an on-line process that may be helpful in developing a physically-meaningful empirical model. Future work must explore methods for obtaining aspects of the proposed control law (e.g., $\hat{V}$) on-line, for determining how to reliably design objective functions or constraints that are conducive to obtaining desired data, and for determining on-line what type of data is desirable.

## REFERENCES


Alanqar, A., Durand, H., and Christofides, P.D. (2015a). On identification of well-conditioned nonlinear systems: Application to economic model predictive control of nonlinear processes. *AIChE Journal*, 61, 3353–3373.

Alanqar, A., Ellis, M., and Christofides, P.D. (2015b). Economic model predictive control of nonlinear process systems using empirical models. *AIChE Journal*, 61, 816–830.

Brunton, S.L., Proctor, J.L., and Kutz, J.N. (2016). Discovering governing equations from data by sparse identification of nonlinear dynamical systems. *Proceedings of the National Academy of Sciences*, 113, 3932–3937.

Ellis, M., Durand, H., and Christofides, P.D. (2014). A tutorial review of economic model predictive control methods. *Journal of Process Control*, 24, 1156–1178.

Heidarinejad, M., Liu, J., and Christofides, P.D. (2012). Economic model predictive control of nonlinear process systems using Lyapunov techniques. *AIChE Journal*, 58, 855–870.

Heirung, T.A.N., Foss, B., and Ydstie, B.E. (2015). MPC-based dual control with online experiment design. *Journal of Process Control*, 32, 64–76.

Houska, B., Telen, D., Logist, F., and Impe, J. (2017). Self-reflective model predictive control. *SIAM Journal on Control and Optimization*, 55, 2959–2980.

Larsson, C.A., Annergren, M., Hjalmarsson, H., Rojas, C.R., Bombois, X., Mesbah, A., and Modén, P.E. (2013). Model predictive control with integrated experiment design for output error systems. In *Proceedings of the European Control Conference*, 3790–3795. Zürich, Switzerland.

Ljung, L. (1999). *System Identification: Theory for the User*. Prentice Hall PTR, Upper Saddle River, NJ.

Marafioti, G., Bitmead, R.R., and Hovd, M. (2014). Persistently exciting model predictive control. *International Journal of Adaptive Control and Signal Processing*, 28, 536–552.

Mhaskar, P., Liu, J., and Christofides, P.D. (2013). *Fault-Tolerant Process Control: Methods and Applications*. Springer-Verlag, London, England.

Müller, M.A. and Allgöwer, F. (2017). Economic and distributed model predictive control: Recent developments in optimization-based control. *SICE Journal of Control, Measurement, and System Integration*, 10, 39–52.

Muñoz de la Peña, D. and Christofides, P.D. (2008). Lyapunov-based model predictive control of nonlinear systems subject to data losses. *IEEE Transactions on Automatic Control*, 53, 2076–2089.

Qin, J. and Badgwell, T. (2003). A survey of industrial model predictive control technology. *Control Engineering Practice*, 11, 733–764.

Rawlings, J.B., Angeli, D., and Bates, C.N. (2012). Fundamentals of economic model predictive control. In *Proceedings of the IEEE Conference on Decision and Control*, 3851–3861. Maui, Hawaii.

Sontag, E.D. (1989). A 'universal' construction of Artstein's theorem on nonlinear stabilization. *Systems & Control Letters*, 13, 117–123.