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Selection of Control Configurations for Economic Model Predictive Control Systems

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Economic model predictive control (EMPC) is a feedback control method that dictates a potentially dynamic (time-varying) operating policy to optimize the process economics. The objective function used in the EMPC system may be a general nonlinear function that describes the process/system economics. As this function is not derived on the sole basis of classical control considerations (stabilization, tracking, and optimal control action calculation) but rather on the basis of economics, selecting the appropriate control configuration, and quantifying the influence of a given input on an economic cost is an important task for the proper design and computational efficiency of an EMPC scheme. Owing to these considerations, an input selection methodology for EMPC is proposed which utilizes the relative degree and the sensitivity of the economic cost with respect to an input to identify and select stabilizing manipulated inputs with the most dynamic and steady-state influence on the economic cost function to be assigned to EMPC. Other considerations for input selection for EMPC are also discussed and integrated into a proposed input selection methodology for EMPC. The control configuration selection method for EMPC is demonstrated using a chemical process example. © 2014 American Institute of Chemical Engineers *AIChE J*, 60: 3230–3242, 2014

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Introduction

Control structure design (i.e., the selection of manipulated, controlled, and measured variables) has been the subject of extensive research within the process control community for many years resulting in many methods for input–output loop pairing and control configuration selection (see, for instance, Refs. 1–6). For linear systems, an important early result was the relative gain array (RGA) which is commonly used for input–output loop pairing,[7] particularly in the context of proportional-integral-derivative (PID) control. Several extensions and variations of the RGA have since been proposed like the extension of the RGA to nonsquare linear systems (i.e., systems with a different number of inputs than the number of outputs)[8] and the various extensions of RGA to nonlinear systems.[9,10] Two metrics are often used to evaluate conventional control structure configurations (e.g., control structures consisting of decentralized PID control loops): the open-loop and/or closed-loop process economics and controllability analysis.[11–14] Another potentially important factor in control configuration evaluation may be proper controlled variable (CV) selection. In particular, Skogestad[15] used and mathematically formalized the concept of self-optimizing control, originally proposed by Luyben in 1988,[16] which is a methodology for determining CVs such that when the selected CVs are maintained at their desired set points, nearly (economically) optimal steady-state operation results with an acceptable loss in the presence of disturbances.[15,17,18] Many of the proposed control structure selection methodologies use optimization-based techniques especially mixed-integer optimization problems.[13,14,19,20] One such example is the so-called back-off methodology which consists of solving a mixed-integer optimization program using linearized steady-state process models.[14,19,21]

Most of the control structure selection methodologies have been developed using linear steady-state or dynamic process models with the assumption that the system is to be operated at steady-state (i.e., the main control objective is to force the system to the desired operating steady-state and maintain operation at this state in the presence of disturbances). Within the context of dynamic operation of nonlinear systems, fewer results and methodologies on control structure selection exist that explicitly consider the process dynamics and nonlinearities. One simple and potentially effective

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method for evaluating control configurations of multivariable nonlinear systems is to use a relative degree analysis which may be useful as the relative degree is essentially a measure of the directness of the effect of an input on an output or the physical closeness between an input and an output.[22]

One control scheme that may operate the system in a possibly dynamic fashion (i.e., forced dynamic operation) is economic model predictive control (EMPC) which is a nonlinear predictive control scheme that optimizes an objective function describing the process economics[23–31] (see also Ref. 32 for an overview of recent results on EMPC). In the case of tracking model predictive control (MPC) formulated with a quadratic cost function (i.e., $x^T Q_c x + u^T R_c u$ where Q_c and R_c are positive definite matrices), the weighting matrices Q_c and R_c are typically tuned such that all the inputs have a direct effect on the cost function. For EMPC, however, not all of the possible manipulated inputs must have a direct effect on the economic cost of the EMPC as it is not derived from traditional control objectives. As a consequence, control configuration selection for EMPC (i.e., which inputs to manipulate for a given EMPC cost) is an open and relevant problem. Since EMPC may dictate a dynamic operating policy, the system may be operated in a larger region of operation (i.e., the effect of nonlinearities in the process may become significant) compared to traditional/conventional control schemes which force the system to operate in a small neighborhood of the steady-state. Thus, traditional methods that evaluate control structures on the basis of steady-state operation using linear or linearized models may not provide sufficient results within the context of EMPC. Furthermore, owing to the fact that EMPC may use a general nonlinear objective function, solving EMPC is generally more computationally challenging compared to tracking MPC. Therefore, proper input selection for EMPC may also have implications in the computational burden of the EMPC optimization problem as the optimization may be poorly conditioned when the economic cost has a weak dependence on some of the manipulated inputs (i.e., the decision variables of the optimization problem).

Owing to the aforementioned considerations, a methodology for control configuration selection for EMPC is proposed. Treating the economic cost function as the output, a relative degree analysis is completed to determine which inputs have the most direct dynamic effect on the economic cost. The choice of inputs that are controlled by EMPC are the inputs that have a low relative degree with respect to the cost function (typically, one or two). The remaining possible inputs are partitioned to the set of inputs controlled by EMPC and the set of remaining inputs that are not controlled by EMPC on the basis of a sensitivity analysis and a relative degree analysis of any known disturbances. Furthermore, the set of inputs selected for EMPC is ensured to be a stabilizing one. The remaining inputs not controlled by EMPC may be held constant if the control configuration selected has a sufficient degree of robustness or they may be manipulated through other control systems (i.e., outside of EMPC). An evaluation and analysis of the control configuration selection methodology is provided using a chemical process example.

Preliminaries

Notation. *The norms $|\cdot|$ and $|\cdot|_Q$ denote the Euclidean norm of a vector and the square of the weighted Euclidean norm of a vector, where Q is a positive definite matrix (i.e., $|x|_Q = x^T Q x$), respectively. The symbol $S(\Delta, N)$ denotes the family of piecewise constant, right-continuous functions with period Δ over the time interval $N\Delta$ (i.e., $u(t) \in S(\Delta, N)$ means that $u(t) = u_i$ for all $t \in [\tau_i, \tau_{i+1})$ for $i = 0, 1, \ldots, N-1$ where u_i is a constant, $\tau_i = t_0 + i\Delta$, and t_0 is the initial time). The symbol Ω_ρ denotes a level set of a function $V(x)$ (i.e., $\Omega_\rho := \{x \in \mathbf{R}^{n_x} : V(x) \leq \rho\}$). A function $\alpha_i : [0, a) \to [0, \infty)$ is said to be of class $\mathcal{K}$ if it is continuous, strictly increasing, and $\alpha(0) = 0$. The notation $L_f h(x)$ denotes the Lie derivative of the scalar field $h(x)$ along the vector field $f(x)$, that is*

$$L_f h(x) = \frac{\partial h(x)}{\partial x} f(x)$$

It is also important to recall the following two types of Lie derivatives

$$L_g L_f h(x) = \frac{\partial (L_f h)}{\partial x} g(x)$$

$$L_f^k h(x) = L_f \left(L_f^{k-1} h(x) \right) = \frac{\partial (L_f^{k-1} h)}{\partial x} f(x)$$

where $g(x)$ is a vector field.

Class of nonlinear systems

The class of input-affine nonlinear systems considered have the following state-space form

$$\dot{x}(t) = f(x(t)) + \sum_{j=1}^{n_u} g_j(x(t)) u_j(t) + \sum_{i=1}^{n_w} w_i(x(t)) d_i(t) \tag{1}$$

where $x \in \mathbf{R}^{n_x}$ is the state vector, $u \in U \subseteq \mathbf{R}^{n_u}$ is the input vector consisting of all possible manipulated inputs, and $d \in W \subseteq \mathbf{R}^{n_w}$ is the disturbance vector. The input and disturbance vectors are bounded in the following sets

$$U = \{u \in \mathbf{R}^{n_u} : u_{\min} \preceq u \preceq u_{\max}\} \tag{2}$$

$$W = \{d \in \mathbf{R}^{n_w} : |d| \leq w_b\} \tag{3}$$

where the symbol $\preceq$ denotes a component-wise inequality, $u_{\min}, u_{\max} \in \mathbf{R}^{n_u}$ denote the minimum and maximum allowable control actions, and w_b bounds the norm of the disturbance vector. The vector functions f, g_j for $j = 1, \ldots, n_u$, and w_i for $i = 1, \ldots, n_w$ are sufficiently smooth vector functions on $\mathbf{R}^{n_x}$. The existence of a time-invariant economic cost (scalar) function given by $l_e(x,u)$, which is a sufficiently smooth function of its arguments, is assumed for the system of Eq. 1. For reasons explained below, we assume the economic cost function has the following form

$$l_e(x, u) = l_{e,x}(x) + l_{e,u}(u) \tag{4}$$

This assumption may be relaxed which will be also discussed below. Additionally, economic constraints are imposed and are assumed to have the following form

$$\int_{t_0}^{t_f} g_e(x(t), u(t)) dt \leq 0 \tag{5}$$

where $x(t)$ is the solution to Eq. 1 with a specified input trajectory $u(t)$ over the time $t = t_0$ to $t = t_f$. Examples of constraints that have the form of Eq. 5 include constraints that limit the average amount of reactant material that can be fed to a reactor over the operation period t_0 to t_f and constraints on the average production rate of the desired product.

The state vector is assumed to be measured synchronously at sampling times $\tau_k = t_0 + k\Delta,\ k = 0,1,\ldots$ where t_0 is the initial time and Δ is the sampling period. EMPC computes sample-and-hold (i.e., zeroth-order hold) control actions with a sampling period Δ for the continuous-time system of Eq. 1. Thus, the closed-loop system of Eq. 1 under EMPC forms a closed-loop sampled-data system with control actions

$$u(t)=\kappa(x(\tau_k)) \text{ for } t \in [\tau_k, \tau_{k+1}) \tag{6}$$

where $\kappa(x(\tau_k))$ is the implicit control law resulting from the EMPC scheme which is described below.

Economic model predictive control

EMPC schemes are MPC schemes formulated with an objective function that reflects the process/system economics. The optimization problem that defines the EMPC has the following form

$$\max_{u\in S(\Delta,N)} \int_0^{\tau_N} l_e(\tilde{x}(t), u(t))dt \tag{7a}$$

$$\text{s.t.} \quad \dot{\tilde{x}}(t)=f(\tilde{x}(t))+\sum_{j=1}^{n_u} g_j(\tilde{x}(t))u_j(t) \tag{7b}$$

$$\tilde{x}(0)=x(\tau_k) \tag{7c}$$

$$u(t) \in U, \forall t \in [0, \tau_N) \tag{7d}$$

$$\tilde{x}(t) \in \mathcal{X} \tag{7e}$$

$$\int_0^{\tau_N} g_e(\tilde{x}(t), u(t))dt \le 0 \tag{7f}$$

where the decision variable $u(t)$ of the optimization problem is the piecewise constant input trajectory over the finite-time prediction horizon. The notation $\tilde{x}(t)$ denotes the predicted state trajectory of the nominal closed-loop system (Eq. 1 with $d(t) \equiv 0$) with the input trajectory computed by the EMPC.

In the optimization problem of Eq. 7, the objective function of Eq. 7a represents the operating profit (cost) of the process/system of Eq. 1 which the EMPC maximizes (minimizes) over the prediction horizon through dynamic operation. The nominal model of the process/system is used to predict the future behavior of the process/system (i.e., the constraint of Eq. 7b). The nominal model is initialized with a state measurement $x(\tau_k)$ obtained at the current sampling time (Eq. 7c). The input constraint of Eq. 7d ensures that the computed control actions be within the set of admissible inputs U. Owing to the finite length prediction horizon of the EMPC, stability constraints are typically used in the formulation of the EMPC to ensure a form of stability of the closed-loop system. The stability constraints are expressed by Eq. 7e which forces the solution $\tilde{x}(t)$ to the model of Eq. 7b under the input trajectory computed by the EMPC be in some set. Various constraints have been proposed in the literature including various terminal region constraints[24,25] and stability constraints designed via Lyapunov-based control techniques[27] (see, for instance, Ref. 32 for an overview of the various types of stability constraints). Depending on the type of stability constraint and/or to improve closed-loop performance under the EMPC, a terminal penalty (i.e., $-V_T(\tilde{x}(\tau_N))$) may be added to the objective function of the EMPC.[24] Besides the economic objective function, another key difference that separates EMPC from traditional control structures (e.g., tracking MPC) is the use of economics-based constraints (Eq. 7f) directly imposed on the computed input trajectory.

The EMPC is implemented in a receding horizon fashion. At any sampling instance τ_k, the EMPC receives a state measurement $x(\tau_k)$ and solves the optimization problem of Eq. 7. The optimal input trajectory computed over the prediction horizon of EMPC is denoted as $u^*(t|\tau_k)$ and is defined for $t \in [0,\ \tau_N)$. The control action computed for the first sampling period is sent to the control actuators to be applied over the sampling period τ_k to $\tau_{k+1}=\tau_k+\Delta$. The input trajectory applied to the system of Eq. 1 under EMPC is given by

$$u(t)=u^*(0|\tau_k) \tag{8}$$

for $t \in [\tau_k, \tau_{k+1}), k=0, 1, \ldots$

Remark 1. *Rigorous stability proofs and algorithms for guaranteed performance under EMPC have been proposed,*[23–29,31] *but this is not the focus of this article. Furthermore, the proposed input selection methodology may be applied to any EMPC formulation or algorithm.*

Remark 2. *The objective function of Eq.* 7a *is often referred to as the economic cost function to maintain consistency with tracking MPC, where the quadratic cost function is typically referred to as the performance index or cost. However, the economic cost function could represent an operating profit (as is the case in this work) or operating cost depending on the application and the economic performance metric of the particular application.*

Input Selection for EMPC

In this section, the input selection methodology for EMPC is presented. In the next four subsections, the analysis techniques that are used in the methodology are described which include: determining the relative degree of the economic cost with respect to the inputs, computing the dynamic sensitivity of the economic cost, computing the steady-state sensitivity of the economic cost, and imposing a stabilizability requirement on the final input selection for EMPC. The last subsection summarizes the input selection methodology.

The next three subsections propose analysis techniques to quantify the sensitivity of the economic cost with respect to inputs. To this end, it is important to point out the difference between EMPC and MPC. Recall, quadratic cost functions used in tracking MPC have the form

$$\int_0^{\tau_N} \left(|\tilde{x}(t)|_{Q_c}+|u(t)|_{R_c}\right)dt \tag{9}$$

where Q_c and R_c are positive definite weighting matrices and thus, the cost function is sensitive to all the inputs, that is, the decision variables of a tracking MPC optimization problem (i.e., the input trajectory) have a direct effect on the second quadratic term of the cost function as well as an indirect impact on the first term through the dynamic model. Conversely, EMPC is formulated with the economic cost function $l_e(x,u)$. As the economic cost function is typically derived from the process economics, it may not be sensitive to all of the available inputs.

Several issues may arise when the economic cost is not sensitive to some of the inputs. First, the optimization problem may be more difficult to solve because, for instance, the optimization problem may be ill-conditioned if an input has little effect (i.e., low sensitivity) on the economic cost function (see, for example, Ref. 33 for challenges arising in the context of ill-conditioned optimization problems). Second, the effect of plant-model mismatch may be significant when the economic cost is not as sensitive to an input. For instance, large input changes are needed to influence the cost for inputs with a modeled weak dependence. This makes the optimal solution sensitive to plant-model mismatch (the actual sensitivity of the economic cost with respect to the input may be significantly greater/lower). Third, if an input does not influence the economic cost function much, it may be desirable to decouple this input from the EMPC problem to reduce the computational burden required for solving the optimization problem on-line by either fixing the input to its nominal value or economically optimal steady-state value or by computing its control action through other control systems (e.g., proportional-integral control, or tracking MPC).

Relative degree of cost to inputs

Motivated by the fact that EMPC optimizes the process dynamics with respect to the economic cost which may lead to dynamic operation, one method for carrying out input selection for EMPC is to consider the time evolution of the economic cost along the process dynamics. Then, select the inputs that have more direct impact on the time evolution of the economic cost. In other words, consider the time derivative of the economic cost function

$$\frac{dl_e(x,u)}{dt} = \frac{\partial l_{e,x}}{\partial x}\frac{dx}{dt} + \frac{\partial l_{e,u}}{\partial u}\frac{du}{dt} \tag{10}$$

where the elements in the term $\partial l_{e,u}/\partial u$ are non-zero for any inputs that explicitly appear in the economic cost. As the input trajectory is a piecewise constant function, the second term of the right-hand side of Eq. 10 is neglected (with this analysis these inputs should be placed on EMPC since they explicitly appear in the economic cost).

The vector field of Eq. 1 with $d(t) \equiv 0$ can be substituted into Eq. 10 which yields

$$\frac{\partial l_{e,x}(x)}{\partial x}\left(f(x)+\sum_{j=1}^{n_u} g_j(x)u_j\right) = : L_f l_{e,x} + \sum_{j=1}^{n_u} L_{g_j} l_{e,x} u_j(t) \tag{11}$$

where $L_f l_{e,x}(x)$ and $L_{g_j} l_{e,x}(x)$ denote the Lie derivatives of $l_{e,x}$ along vector fields $f(x)$ and $g_j(x)$, respectively. If $L_{g_j} l_{e,x}(x) \not\equiv 0$, the jth input does not have a direct effect on economic cost (in terms of the first derivative). Due to the coupled nature of the dynamics, the jth input may still influence the economic cost through higher-order derivatives. Therefore, we define the relative degree or relative order r_j of the economic cost with respect to the jth input as the smallest positive integer that satisfies

$$\begin{aligned} L_{g_j} L_f^{k-1} l_{e,x}(x) &\equiv 0, \; k=1, \; 2, \; \ldots, \; r_j-1, \\ L_{g_j} L_f^{r_j-1} l_{e,x}(x) &\not\equiv 0 \end{aligned} \tag{12}$$

or $r_j=\infty$ if no such integer exists. By convention, the relative degree of the economic cost with respect to any input with $\partial l_{e,u}/\partial u \not\equiv 0$ is zero. Here, the relative degree is similar to standard input–output analysis for nonlinear systems[34–36] where the economic cost function is treated as an output. It is important to point out that the scalar fields $l_{e,x}(x), L_f l_{e,x}(x), \ldots, L_f^{r_j-1} l_{e,x}(x)$ are linearly independent.[35] As $\mathbf{R}^{n_x}$ can only have n_x linearly independent elements, $r_j \leq n_x$ if r_j is finite. Additionally, for disturbances that are explicitly included in the process model, one may be able to compute the relative degree of the economic cost with respect to these disturbances. This may be helpful in the input selection methodology for EMPC (see the "Input Selection Methodology" subsection later).

Since the relative degree is essentially a measure of how fast the input affects the process economics, the relative degree analysis allows for some intuition of how manipulating the jth input affects the time evolution of the economic cost. This is of particular interest when EMPC dictates a time-varying or dynamic operating policy (i.e., off steady-state operation). Using the relative degree as a basis, a systematic method for selecting the manipulated inputs for which EMPC computes control actions can be developed while explicitly accounting for the dynamics of the system. If the relative degree of the jth input is large (i.e., the jth input influences high-order derivatives with respect to each input; perhaps, third-order or higher time derivatives of the economic cost), using EMPC to compute control actions for the jth input may not be effective with respect to the closed-loop economic performance and/or computationally efficient.

Remark 3. *It may be possible to consider more general cost functions other than the ones of the assumed form (i.e., $l_e(x,u)=l_{e,x}(x)+l_{e,u}(u)$). In this case, for any inputs where $\partial l_e/\partial u_j, j=1,\ldots,n_u$ is non-zero (i.e., any inputs explicitly appearing in the economic cost function), these inputs have a direct effect on the economic cost. One could still determine the relative degree of the other inputs by taking the inputs appearing in the cost function as fixed parameters to determine the relative degree. It is important to note that one type of cost function that possesses the assumed form is a quadratic cost function. The economic cost functions in the examples considered in this work all have the assumed form. Also, the relative degree analysis could be applied to a time-varying cost function (i.e., $l_e(t,x,u)=l_{e,x}(t,x)+l_{e,u}(t,u)$ which is an explicit function of the time) when the cost function is a continuous or piecewise continuous function of time by generalizing the definition of Lie derivative to time-varying vector fields. However, other issues arise when using a time-varying cost function and as a result, using an EMPC scheme that explicitly accounts for this time variation may be important to achieve the best possible closed-loop performance under EMPC; see, for instance, Ref. 37 for details on this point.*

Connection Between Relative Degree and a Directed Graph. For large-scale process networks, analytical computation of the relative degree may become tedious. However, one may use the directed graph method for determining the relative degree.[22,38] This methodology has the advantage that only structural information of the process model is required. In the context of this work, the output is considered to be the economic cost. The edges are constructed using the following modified rules based on Ref. 22 to treat the economic cost as the output:

1. If $\partial f_i(x)/\partial x_k \not\equiv 0$ for $i = 1,\ldots, n_x$ and $k = 1,\ldots,n_x$, then there is an edge from x_k to x_i.
2. If $g_{j,k}(x) \not\equiv 0$ for $k = 1,\ldots, n_x$ and $j = 1,\ldots,n_u$, then there is an edge from u_j to x_k.
3. If $\partial l_e(x,u)/\partial x_i \not\equiv 0$ for $i = 1,\ldots, n_x$, then there is an edge from x_i to l_e.
4. If $\partial l_e(x,u)/\partial u_j \not\equiv 0$ for $j = 1,\ldots, n_u$, then there is an edge from u_j to l_e.

where $f_k(x)$ and $g_{j,k}(x)$ denote the kth elements of the vector fields $f(x)$ and $g_j(x)$, respectively. If there are known disturbances, the disturbance may be treated as an input in the above directed graph rules.

Utilizing the first main result from Ref. 22, a connection between the relative degree as defined in Eq. 12 and the directed graph constructed with the rules presented above can be made. Defining the length of shortest path connecting the jth input to the economic cost (i.e., the smallest number of edges connecting the jth input to the economic cost) as L_j, the relative degree of the jth input with respect to the economic cost is $r_j = L_j - 1$. It is important to point out that this works for many cases. However, there are cases where this does not work like cases where there are potential cancellations (see Ref. 22 for more details on this point). This gives a rather intuitive understanding of how the inputs affect the economic cost. Furthermore, it requires only limited structural understanding of the process dynamics (i.e., not detailed process models) during the input selection phase of the control structure design. For instance, consider the following example.

Example 1. *Consider the following input-affine nonlinear system*

$$\begin{aligned} \dot{x}_1 &= f_1(x_2, x_3) + g_{1,1}(x)u_1 \\ \dot{x}_2 &= f_2(x_1, x_2) \\ \dot{x}_3 &= f_3(x_1, x_3) + g_{2,3}(x)u_2 \end{aligned} \tag{13}$$

where the vector fields are $f^T(x) = [f_1(x_2, x_3)\ f_2(x_1, x_2)\ f_3(x_1, x_3)]$, $g_1^T(x) = [g_{1,1}(x)\ 0\ 0]$, and $g_2^T(x) = [0\ 0\ g_{2,3}(x)]$ and the economic cost function has the following form

$$l_e(x, u) := \hat{l}_{e,x}(x_2) + \hat{l}_{e,u}(u_2) \tag{14}$$

The relative degree of the economic cost with respect to u_2 is defined to be 0 as the economic cost is an explicit function of this input. For the input u_1, the Lie derivative of $l_e(x,u)$ along the vector field $g_1(x)$ is

$$L_{g_1} l_e = \frac{\partial l_e}{\partial x} g_1(x) \equiv 0 \tag{15}$$

Since the first Lie derivative is zero, higher order Lie derivatives are computed. The next Lie derivative is

$$L_{g_1} L_f l_e = \frac{\partial}{\partial x_1} \left[\frac{\partial l_e}{\partial x_2} f_2(x_1, x_2) \right] g_{11}(x) \not\equiv 0 \tag{16}$$

From this analysis, the relative degree of the economic cost function with respect to the input u_1 is 2.

Applying the construction rules for the nodes and edges, the directed graph for the system of Eq. 13 is displayed in Figure 1. From the directed graph, one can easily determine the relative degree. The shortest path between the input u_1 and the economic cost is 3. Therefore, the relative degree of the economic cost with respect to u_1 is 2. Similarly, the shortest path from the input u_2 to the economic cost is 1, so, the relative degree is 0. The relative degrees computed from the directed graph agree with the ones computed analytically.

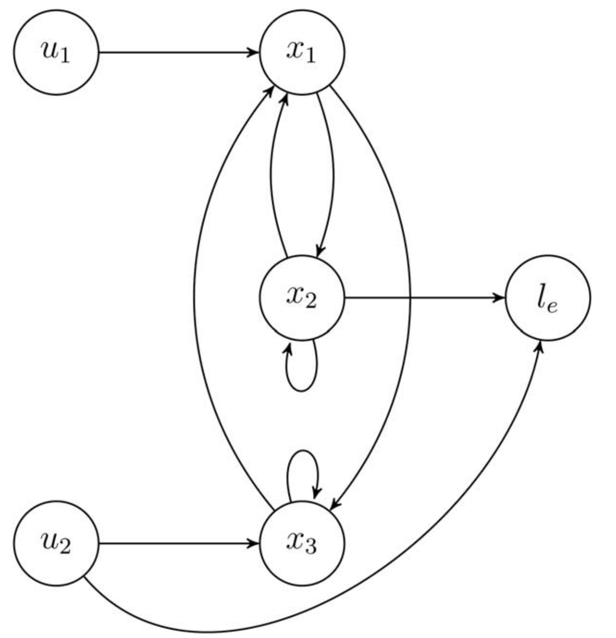

Figure 1. Directed graph representing the system of Eq. 13.

Dynamic sensitivity of the economic cost

While the relative degree is a readily computable metric that quantifies the directness of the effect of an input on the economic cost, it is unable to capture the magnitude of the interaction between an input and the economic cost.[22] One cannot distinguish the degree of the sensitivity of the economic cost with respect to inputs of the same relative degree. In linear systems, the steady-state gain on the economic cost with respect to an input is one metric that captures such a sensitivity. However, the steady-state gain is state dependent for nonlinear systems in general. Therefore, in this subsection, an analysis technique to quantify the dynamic sensitivity of the economic cost with respect to an input is proposed.

For dynamic sensitivity analysis, we consider the inputs with the same relative degree. Let $\hat{u} \in \mathbf{R}^{n_r}$ be a vector containing all inputs with relative degree r. The inputs with relative degree not equal to r are taken as constants in this analysis set to their economically optimal value and are incorporated in the $f(x)$ term of the model of Eq. 1. To avoid potential scaling differences of inputs which may potentially skew the sensitivity analysis, all inputs contained in the vector $\hat{u}$ are scaled so that $\hat{u}_j \in [-1, 1]$ for $j = 1, \ldots, n_r$. The auxiliary scalar output variable $y(t)$ is defined as the state-dependent part of the economic cost $y(t) = l_{e,x}(x(t))$. Consider a Taylor series expansion of $y(t)$ at a time t^*

$$y(t) = \sum_{k=0}^{\infty} \frac{(t-t^*)^k}{k!} \frac{d^k y(t^*)}{dt^k} \tag{17}$$

The kth derivative of y for $k = 0, 1, \ldots, r-1$ is

$$\frac{d^k y(t^*)}{dt^k} = L_f^k l_{e,x}(x(t^*)) \tag{18}$$

and the rth derivative of y is

$$\frac{d^r y(t^*)}{dt^r} = L_f^r l_{e,x}(x(t^*)) + \sum_{j=1}^{n_r} L_{g_j} L_f^{r-1} l_{e,x}(x(t^*)) \hat{u}_j(t^*) \tag{19}$$

Thus, the Taylor series expansion can be written as

$$\begin{aligned} y(t) = &\sum_{k=0}^{r} \frac{(t-t^*)^k}{k!} L_f^k l_{e,x}(x(t^*)) \\ &+ \frac{(t-t^*)^r}{r!} \sum_{j=1}^{n_r} L_{g_j} L_f^{r-1} l_{e,x}(x(t^*)) \hat{u}_j(t^*) \\ &+ \sum_{k=r+1}^{\infty} \frac{d^k y(t^*)}{dt^k} \frac{(t-t^*)^k}{k!} \end{aligned} \tag{20}$$

The high-order ($r+1$ order and higher) derivatives of y are neglected to obtain an approximation of $y(t)$

$$y(t) \approx \sum_{k=0}^{r} \frac{(t-t^*)^k}{k!} L_f^k l_{e,x}(x(t^*)) + \frac{(t-t^*)^r}{r!} \sum_{j=1}^{n_r} L_{g_j} L_f^{r-1} l_{e,x}(x(t^*)) \hat{u}_j(t^*) \tag{21}$$

Consider the difference of the output $\Delta y(t) = y_1(t) - y_2(t)$ with respect to a change $\Delta \hat{u}_j(t^*) = \hat{u}_{j,1}(t^*) - \hat{u}_{j,2}(t^*)$ and all other inputs constant. From Eq. 21, the following can be derived

$$\left.\frac{\Delta y}{\Delta u_j}\right|_{\Delta u_k, k \neq j} = \frac{(t-t^*)^r}{r!} L_{g_j} L_f^{r-1} l_{e,x}(x(t^*)) \tag{22}$$

Therefore, the n_r-dimensional vector S_r is defined with elements

$$S_{r,j} := L_{g_j} L_f^{r-1} l_{e,x}(x(t^*)) \tag{23}$$

for $j = 1, \ldots, n_r$. The vector S_r contains elements that essentially quantify the dynamic sensitivity of inputs with the same relative degree on the economic cost. To use the sensitivities in a comparison, they are normalized with respect to the Euclidean norm

$$\bar{S}_{r,j} := \frac{S_{r,j}^2}{|S_r|^2} = \frac{S_{r,j}^2}{\left(\sum_{j=1}^{n_r} S_{r,j}^2\right)} \tag{24}$$

and $\bar{S}_{r,j} \in [0,1]$. The economic cost is more sensitive to inputs whose corresponding $\bar{S}_{r,j}$ values are close to one compared to inputs with corresponding $\bar{S}_{r,j}$ values close to zero. Thus, the dynamic sensitivity analysis ranks inputs with the same relative degree on the basis of their dynamic sensitivities. Also, $\bar{S}_{r,j}$ may be computed for various points in state-space to capture the dynamic sensitivities (i.e., sensitivity of the economic cost with respect to inputs for states off steady-state).

Example 2. *Consider a nonisothermal continuous stirred tank reactor (CSTR), where an elementary second-order reaction of the form $A \to B$ occurs. The states of the CSTR are the reactor temperature x_1 and the concentration of A in the reactor which is denoted as x_2 (i.e., the state vector is $x^T = [x_1 \ x_2]$). The evolution of the CSTR system is described by the following ordinary differential equations in dimensionless form*

$$\frac{dx_1}{d\tau} = x_{10} - x_1 - \beta_1 e^{-1/x_1} x_2^2 + \beta_2 + \beta_3 u_1 \tag{25a}$$

$$\frac{dx_2}{d\tau} = -x_2 - \beta_4 e^{-1/x_1} x_2^2 + \beta_5 + u_2 \tag{25b}$$

where the process parameters are $\beta_1 = -1.73 \times 10^5$, $\beta_2 = 1.44 \times 10^{-3}$, $\beta_3 = 1.44 \times 10^{-3}$, $\beta_4 = 5.92 \times 10^6$, and $\beta_5 = 1.14$. The CSTR has two candidate inputs: the heat rate u_1 supplied to the reactor and the inlet concentration of species A to the reactor u_2. Both inputs have been scaled so that $u_j \in [-1, 1]$ for $j = 1, 2$. The production rate of B corresponds to the dominant factor in the operating profit of the CSTR. Thus, the economic cost function is

$$l_e(x, u) = e^{-1/x_1} x_2^2 \tag{26}$$

The relative degree of the economic cost with respect to both inputs is 1, so the relative degree analysis would not be able to discriminate between the importance of controlling each of the inputs with EMPC. The Lie derivatives of $l_{e,x}(x) = l_e(x, u)$ with respect to the vector fields $g_1(x) = [\beta_3 \ 0]^T$ and $g_2(x) = [0 \ 1]^T$ are

$$L_{g_1} l_{e,x}(x) = \frac{\beta_3}{x_1^2} e^{-1/x_1} x_2^2 \tag{27}$$

$$L_{g_2} l_{e,x}(x) = 2 e^{-1/x_1} x_2 \tag{28}$$

From the Lie derivatives, the dynamic sensitivities can be computed. For simplicity of presentation, the Lie derivatives are evaluated at the economically optimal steady-state $x_{1s}^* = 0.08$ and $x_{2s}^* = 0.21$ and the normalized dynamic sensitivity vector for the inputs with relative degree 1 is

$$\bar{S}_1 = [0.0 \ 1.0] \tag{29}$$

This analysis suggests that the input u_2 has a more substantial dynamic effect compared to the input u_1. In terms of input selection for EMPC, it would be more desirable in terms of the dynamic sensitivity analysis to control the input u_2 compared to the input u_1. In fact, it has been demonstrated that periodic switching of the inlet concentration achieves greater production rates compared to a constant inlet concentration equal to the time-average inlet concentration of the periodic switching policy (e.g., Ref. 32). Since the reaction rate is concave with respect to the temperature, the maximum production rate is achieved by supplying the maximum allowable heat rate to the reactor (i.e., little benefit with respect to the economic cost is achieved when the heat rate is controlled by EMPC under nominal operation).

Steady-state sensitivities of the economic cost

From the dynamic sensitivity analysis, the inputs with the same relative degree can be ranked on the basis of the dynamic sensitivity of the economic cost. However, this ranking is made with respect to other inputs with the same relative degree (i.e., the dynamic sensitivity vector $\bar{S}_r$ is normalized with the sensitivity of the other inputs). Therefore, a procedure is needed to identify if the interaction between an input and the economic cost is significant with respect to all the other inputs. To accomplish this, we propose to use a steady-state sensitivity.

The input vector is scaled so that $u_j \in [-1, 1]$ for $j = 1, \ldots, n_u$ to remove any scaling differences between the inputs. A steady-state of the system of Eq. 1, which is denoted as x_s, with its corresponding steady-state input, which is denoted as u_s, satisfies the following algebraic equation

$$f(x_s) + \sum_{j=1}^{n_u} g_j(x_s) u_{s,j} = 0 \tag{30}$$

For a given steady-state input, the corresponding steady-state can be computed, and thus, we can write: $x_s = \bar{f}(u_s)$ where $\bar{f} : \mathbf{R}^{n_u} \to \mathbf{R}^{n_x}$ maps a given steady-state input to a corresponding steady-state. With $x_s = \bar{f}(u_s)$, the state dependence on the steady-state economic cost can be removed: $l_e(x_s, u_s) = l_e(\bar{f}(u_s), u_s) \equiv \bar{l}_e(u_s)$. The steady-state sensitivity on the economic cost to the jth input is determined numerically by

$$\frac{\partial \bar{l}_e}{\partial u_{s,j}} \approx \frac{1}{2\delta} [(\bar{l}_e(u_{s,1}, \ldots, u_{s,j-1}, u_{s,j} + \delta, u_{s,j+1}, \ldots, u_{s,n_u}) - \bar{l}_e(u_{s,1}, \ldots, u_{s,j-1}, u_{s,j} - \delta, u_{s,j+1}, \ldots, u_{s,n_u})] \tag{31}$$

where $\delta > 0$ is a small perturbation term. Similar to the dynamic sensitivity analysis, the steady-state sensitivity is normalized with respect to the other inputs

$$\hat{S}_j = \left(\frac{\partial \bar{l}_e}{\partial u_{s,j}}\right)^2 \Bigg/ \left|\frac{\partial \bar{l}_e}{\partial u_s}\right|^2 = \left(\frac{\partial \bar{l}_e}{\partial u_{s,j}}\right)^2 \left(\sum_{j=1}^{n_u}\left(\frac{\partial \bar{l}_e}{\partial u_{s,j}}\right)^2\right)^{-1} \tag{32}$$

where $\hat{S}_j$ will be approximately one for any inputs with a large steady-state sensitivity on the economic cost and will be approximately zero for any inputs with a small steady-state sensitivity on the economic cost.

Stabilizability of control configurations

The aforementioned analysis techniques identify the inputs that influence the economic cost function, but they do not explicitly consider control considerations like controllability and stabilizability. Before a final input selection for EMPC can be made, a verification of such control considerations must be completed. Below, one stabilizability assumption is given which is verifiable for nonlinear systems of the form of Eq. 1. If this assumption is satisfied, a specific formulation of EMPC may be applied to the closed-loop system of Eq. 1 and the closed-loop system will have guaranteed stability properties. Other EMPC formulations that require other types of controllability/stabilizability assumptions (e.g., weak controllability) could be used instead of the assumption and the EMPC formulation provided below.

Lyapunov-Based EMPC. Without loss of generality, the origin of the system of Eq. 1 is assumed to be the steady-state of the unforced system (i.e., $f(0)=0$ with $u(t) \equiv 0$ and $d(t) \equiv 0$). The following assumption is placed on the system of Eq. 1 which is essentially a stabilizability assumption for nonlinear systems.

Assumption. (Existence of a Lyapunov-based Controller). *There exists a Lyapunov-based controller $u=k(x) \in U$ that renders the origin of the nominal closed-loop system of Eq. 1 under $k(x)$ asymptotically stable. This implies that there exists a continuously differentiable Lyapunov function $V(x)$*[36,39] *such that the following holds*

$$\alpha_1(|x|) \le V(x) \le \alpha_2(|x|) \tag{33a}$$

$$\frac{\partial V(x)}{\partial x}\left(f(x)+\sum_{j=0}^{n_u} g_j(x)k(x)\right) \le -\alpha_3(|x|) \tag{33b}$$

$$\left|\frac{\partial V(x)}{\partial x}\right| \le \alpha_4(|x|) \tag{33c}$$

for $x \in D \subseteq \mathbf{R}^{n_x}$ where D is an open neighborhood of the origin where the functions $\alpha_i : [0,a) \to [0,\infty)$, $i=1, 2, 3, 4$ are class $\mathcal{K}$ functions.

It is important to point out that in Assumption 1 the controller $k(x)$ is implemented in a continuous fashion. However, when the controller $k(x)$ is implemented in a sample-and-hold fashion with a sufficiently small sampling period, the origin of the closed-loop system is rendered practically stable (see, for instance, Ref. 40 for details on this point). The stability region under the Lyapunov-based controller is defined as $\Omega_\rho \subseteq D$ which is a level set of $V(x)$ where the time-derivative of the Lyapunov function is negative.

Taking advantage of the explicit Lyapunov-based controller and its corresponding stability region Ω_ρ, the Lyapunov-based economic model predictive control (LEMPC) scheme is characterized by the following optimization problem

$$\max_{u \in S(\Delta,N)} \int_0^{\tau_N} l_e(\tilde{x}(t), u(t))dt \tag{34a}$$

$$\text{s.t.}\ \dot{\tilde{x}}(t)=f(\tilde{x}(t))+\sum_{j=0}^{n_u} g_j(\tilde{x}(t))u_j(t) \tag{34b}$$

$$\tilde{x}(0)=x(\tau_k) \tag{34c}$$

$$u(t) \in U, \forall t \in [0,\tau_N) \tag{34d}$$

$$V(\tilde{x}(t)) \le \tilde{\rho}, \forall t \in [0,\tau_N) \quad \text{if } V(x(t_k)) < \tilde{\rho} \tag{34e}$$

$$\frac{\partial V}{\partial x}\left(f(x(t_k))+\sum_{j=0}^{n_u} g_j(x(t_k))u_j(t_k)\right) \le \frac{\partial V}{\partial x}\left(f(x(t_k))+\sum_{j=0}^{n_u} g_j(x(t_k))k_j(x(t_k))\right) \quad \text{if } V(x(t_k)) \ge \tilde{\rho} \tag{34f}$$

where the LEMPC is a two-mode control strategy with the two modes defined by the Lyapunov-based constraints of Eqs. 34e and 34f.

The design procedure of LEMPC is as follows: (1) an explicit stabilizing controller $k(x)$ is designed for the system of Eq. 1, (2) a Lyapunov function is derived for the closed-loop system under the controller $k(x)$, and (3) the stability region Ω_ρ of the closed-loop system is estimated by taking it to be the (largest) level set of the Lyapunov function such that the time-derivative of the Lyapunov function along the closed-loop state trajectory is negative. For any state starting in Ω_ρ, the existence of an input trajectory that maintains the closed-loop state trajectory in Ω_ρ follows owing to the construction of Ω_ρ. Therefore, one can take advantage of this explicitly defined set in the design of an LEMPC scheme. Namely, the two Lyapunov-based constraints are derived to allow the LEMPC to dynamically operate the system while maintaining operation in Ω_ρ. To accomplish this objective, a subset of Ω_ρ is defined which is denoted as $\Omega_{\tilde{\rho}}$ where $\tilde{\rho} \le \rho$. For any initial state $x(t_k) \in \Omega_{\tilde{\rho}}$, the LEMPC operates in mode 1 operation which enforces that the predicted state trajectory be contained in $\Omega_{\tilde{\rho}}$. For any initial state $x(t_k) \notin \Omega_{\tilde{\rho}}$, the LEMPC operates in mode 2 to force the state into $\Omega_{\tilde{\rho}}$ (i.e., the constraint of Eq. 34f ensures that the time-derivative of the Lyapunov function of the LEMPC is less than the time-derivative of the Lyapunov function under the Lyapunov-based controller). Under the LEMPC, boundedness of the closed-loop state in Ω_ρ is guaranteed for $t \ge t_0$ when $x(t_0) \in \Omega_\rho$. The maximum size of $\Omega_{\tilde{\rho}}$ depends on the properties of a particular system (for more details on the latter point and a rigorous stability analysis of LEMPC, see Ref. 27).

Input selection methodology

The description of the input selection methodology is given in this subsection which is summarized by the flowchart of Figure 2. All the possible manipulated inputs to the system of Eq. 1 are candidate manipulated inputs whose control action may be computed by EMPC. For the remainder of this section, an input on EMPC will refer to an input whose control action is computed by EMPC and an input not on EMPC will refer to an input, that is, fixed or whose control action is computed through another controller. For the latter case, explicit design of an integrated EMPC with

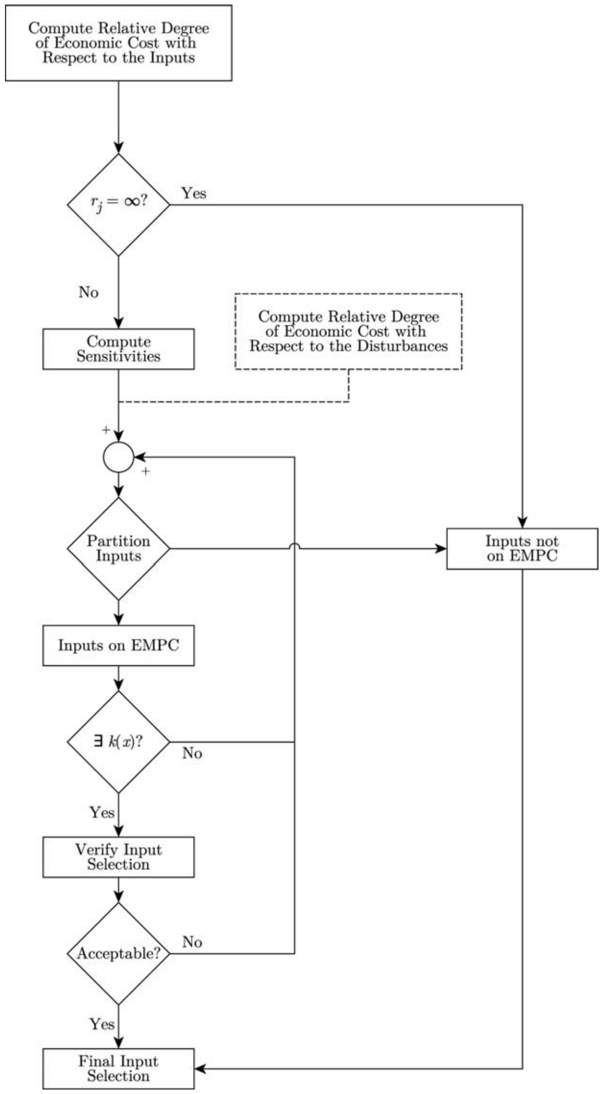

Figure 2. A flowchart of the input selection for EMPC methodology.

Solid lines are used to represent necessary steps and dashed lines are used to represent optional steps.

another controller to compute control actions for the inputs not on EMPC is beyond the scope of the article and thus, only the case where the inputs not on EMPC are fixed to a constant value will be considered in the "EMPC Input Selection for a Chemical Process Example" section below.

The input selection methodology for EMPC is as follows (Figure 2): the relative degree of the economic cost with respect to each candidate input is computed. Any input with an infinite overall relative degree should not be placed on EMPC as these inputs have no influence on the process economics. These inputs can be set to any arbitrary value without adversely affecting the closed-loop economic performance. For the remaining inputs, the inputs with a low relative degree should be on EMPC. Typically, inputs with relative degree 2 or less should be placed on EMPC unless identified otherwise through the sensitivity analysis. When the economic cost function is associated with the outlet product stream of a process network (e.g., the economic cost is the amount of desired product leaving the process), it may be necessary to include more inputs with relative degree greater than 2 owing to closed-loop performance, stability, and robustness considerations.

Several factors may influence the decision on which of the remaining inputs (i.e., inputs with relative degree three or higher) should be on EMPC and to confirm that inputs with relative degree two or lower should be on EMPC. First, the dynamic sensitivities are computed for inputs of the same relative degree which creates a ranking of inputs with the same relative degree on the basis of the dynamic sensitivity of the economic cost. Second, the steady-state sensitivities are computed. If $\bar{S}_{r,j}$ and $\hat{S}_j$ are close to one, the input should be placed on EMPC since it has both a dynamic and a steady-state impact on the economic cost. If $\bar{S}_{r,j}$ and $\hat{S}_j$ are close to zero, the input should not be placed on EMPC since the economic cost is not sensitive with respect to this input. For inputs with $\bar{S}_{r,j}$ close to one and $\hat{S}_j$ close to zero or vice versa, the decision to control these inputs with EMPC should be made on the basis of the remaining two criteria (i.e., relative degree of the economic cost with respect to the disturbances and the stabilizability requirement). It may be desirable from a disturbance rejection standpoint to pick additional inputs that have a smaller relative degree with respect to the cost than the known disturbances. Inputs with $\bar{S}_{r,j}$ close to one and with a low relative degree compared to the disturbances may be chosen to be placed on EMPC. The dynamic sensitivity $\bar{S}_{r,j}$ is used because it quantifies the dynamic sensitivity and EMPC dictates a dynamic operating policy in general to optimize the process economics.

All of the aforementioned factors contribute in partitioning the set of inputs controlled by EMPC and the set of inputs not controlled by EMPC. One must try to find a stabilizing Lyapunov-based controller $k(x)$ with the inputs that will be placed on EMPC. This is a verification step to ensure the selected inputs are able to achieve the stabilizability requirement. If no such controller exists (i.e., it is difficult to find such a controller), then the inputs are repartitioned to include more inputs that will be on EMPC. For this step, the additional inputs to be placed on EMPC should be inputs with the lowest relative degree and highest sensitivity. Once a stabilizing controller is constructed for a certain set of inputs that will be on EMPC, an LEMPC may be formulated for the system and a final verification step is completed. In the final verification step, extensive closed-loop simulations are completed to ensure that the LEMPC scheme has desirable closed-loop properties (e.g., performance, stability, robustness, etc.).

It may be beneficial to use more available inputs as manipulated inputs in the final EMPC control configuration than what is determined from the input selection methodology to increase the overall robustness of the control structure to the effects of disturbances and uncertainty. Two strategies to include more manipulated inputs are: (1) to modify the economic cost (i.e., add quadratic terms) so that these inputs have a more direct effect on the cost function used in the EMPC or (2) to use another controller to compute control actions for the added manipulated inputs instead of setting them to a fixed value (e.g., proportional-integral control may be used to compute the control actions for these inputs). In fact, the former strategy has already been utilized in many EMPC case studies.[25,26,31]

Remark 4. *If there is some flexibility in the choice of economic cost and the sources of the significant disturbances are known (i.e., how the disturbance enters into the process model of Eq.* 1 *is known), one may determine the relative degree of the candidate economic cost functions with respect* *to the disturbances. The economic cost that should be used is the one where the disturbances have a high relative degree compared to the selected manipulated inputs (i.e., the disturbances will have a weaker dynamic effect on the economic cost).*

REMARK 5. *The potential limitations of the proposed methodology for control structure selection for EMPC are: (1) there is no guarantee that there will be a discrete dichotomy between the relative degree of the economic cost and the sensitivities of economic cost with respect to the inputs. For instance, the relative degree analysis may not result in two distinct sets of inputs: one containing the inputs with a low relative degree and another containing the inputs with high relative degree and similarly for the sensitivity analysis. This may make picking the EMPC inputs solely on the basis of these tools difficult. Since the proposed methodology provides tools to identify which inputs to control with EMPC, (2) the final control structure configuration decision is ultimately left to the control engineer (as is the case in many control configuration selection methodologies). Therefore, there is no guarantee that the "optimal" input selection will be selected. However, given the possible uncertainty involved with input selection, it may not be possible to determine the "optimal" input selection. Lastly, (3) closed-loop simulations may be particularly important to select the final input selection from many candidate control configurations. For large-scale systems with many candidate inputs, a large number of simulations may need to be completed to make the final input selection decision given the combinatorial nature of the number of possible control configurations.*

EMPC Input Selection for a Chemical Process Example

In this section, the input selection methodology for EMPC is applied to a chemical process example. Various closed-loop simulation results and analyses are provided to demonstrate the method. The specific example has been chosen as it is manageable to consider all possible combinations of input pairs, while being of sufficient complexity to demonstrate the input selection methodology.

Consider a chemical process example consisting of two CSTRs in series. In each of the reactors a second-order, exothermic reaction of the form $A \rightarrow B$ occurs where A is the reactant material and B is the desired product. Each of the two reactors are fed with fresh reactant material with concentration C_{Aj0} and flow rate F_{j0}, $j=1,\ 2$ where $j=1$ denotes the first CSTR and $j=2$ denotes the second CSTR. To provide heat to the reactor contents, each of the reactors has a heating jacket. The contents of each of the CSTRs have a uniform temperature T_j, concentration of the reactant C_{Aj}, and concentration of the product C_{Bj} for $j=1,\ 2$. Under standard modeling assumptions, the following set of differential equations describing the evolution of the reactor state variables can be derived from first principles modeling techniques

$$\frac{dT_1}{dt}=\frac{F_{10}}{V_1}(T_{10}-T_1)-\frac{\Delta H k_0}{\rho C_p}e^{-E/RT_1}C_{A1}^2+\frac{Q_1}{\rho C_p V_1} \tag{35a}$$

$$\frac{dC_{A1}}{dt}=\frac{F_{10}}{V_1}(C_{A10}-C_{A1})-k_0 e^{-E/RT_1}C_{A1}^2 \tag{35b}$$

$$\frac{dC_{B1}}{dt}=-\frac{F_{10}}{V_1}C_{B1}+k_0 e^{-E/RT_1}C_{A1}^2 \tag{35c}$$

Table 1. Process Parameters of the Reactor–Reactor Process

Notation	Value	Description
T_{10}	300.0 K	CSTR-1 Inlet Temp.
T_{20}	300.0 K	CSTR-2 Inlet Temp.
F_{10}	5.0 $m^3\ h^{-1}$	CSTR-1 Inlet Flow Rate
F_{20}	5.0 $m^3\ h^{-1}$	CSTR-2 Inlet Flow Rate
V_1	1.5 m^3	CSTR-1 Volume
V_2	1.0 m^3	CSTR-2 Volume
k_0	$3.0\times10^4\ m^3 kmol^{-1} h^{-1}$	Pre-exponential Factor
E	3.0×10^4 kJ $kmol^{-1}$	Activation Energy
ΔH	-5.0×10^3 kJ $kmol^{-1}$	Heat of Reaction
C_p	0.231 kJ $kg^{-1}\ K^{-1}$	Heat Capacity
R	8.314 kJ $kmol^{-1}\ K^{-1}$	Gas Constant
ρ_L	1000 kg m^{-3}	Density

$$\frac{dT_2}{dt}=\frac{F_{20}}{V_2}T_{20}+\frac{F_{10}}{V_2}T_1-\frac{(F_{10}+F_{20})}{V_2}T_2 -\frac{\Delta H k_0}{\rho C_p}e^{-E/RT_2}C_{A2}^2+\frac{Q_2}{\rho C_p V_2} \tag{35d}$$

$$\frac{dC_{A2}}{dt}=\frac{F_{20}}{V_2}C_{A20}+\frac{F_{10}}{V_2}C_{A1}-\frac{(F_{10}+F_{20})}{V_2}C_{A2}-k_0 e^{-E/RT_2}C_{A2}^2 \tag{35e}$$

$$\frac{dC_{B2}}{dt}=\frac{F_{10}}{V_2}C_{B1}-\frac{(F_{10}+F_{20})}{V_2}C_{B2}+k_0 e^{-E/RT_2}C_{A2}^2 \tag{35f}$$

where the process parameters are given in Table 1. The possible inputs to the process are the heat rates supplied to the reactors Q_1 and Q_2 and the inlet concentrations of the reactant material C_{A10} and C_{A20}. The available control action is bounded in the following set: $Q_j \in [0.0,\ 100.0]\ \mathrm{MJ\,h^{-1}}, j=1,\ 2$ and $C_{Aj0} \in [0.5,\ 7.5]\ \mathrm{kmol\,m^{-3}}, j=1,\ 2$.

The operating profit of the process is considered to be proportional to the product molar flow rate out of the second reactor. Therefore, the economic cost is

$$l_e(x,u)=(F_{10}+F_{20})C_{B2} \tag{36}$$

where $F_{10}+F_{20}$ is the outlet volumetric flow rate of the second CSTR and C_{B2} is the concentration of the product in the second CSTR. An economics-based constraint is imposed which limits the amount of reactant that may be fed to each reactor

$$\frac{1}{t_f}\int_0^{t_f} F_{j0}C_{Aj0}dt=\dot{M}_{Aj0,\mathrm{avg}} \tag{37}$$

for $j=1{,}2$ where $\dot{M}_{Aj0,\mathrm{avg}}=20\,\mathrm{kmolh^{-1}}$. The average constraint of Eq. 37 is enforced over operating windows of length 0.55 h which has been determined through simulations as the operating window length that leads to improved asymptotic performance of the closed-loop system under EMPC compared to steady-state operation (refer to Ref. 32 for the details for implementing the average constraint over a finite-length operating window). The economically optimal steady-state with respect to the cost of Eq. 36 and the constraint of Eq. 37 corresponds to the economically optimal steady-state input of $Q_1^*=Q_2^*=100\,\mathrm{MJ\,h^{-1}}$ and $C_{A10}^*=C_{A20}^*=4.0\,\mathrm{kmol\,m^{-3}}$ and is open-loop (locally) asymptotically stable.

REMARK 6. *The fact that the economically optimal steady-state is open-loop asymptotically stable implies that there*

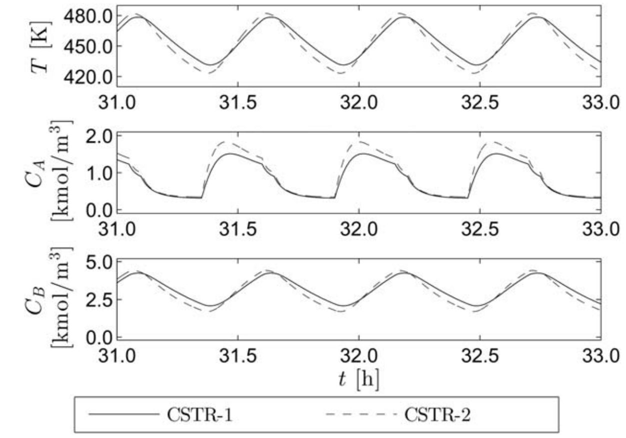

Figure 3. The closed-loop state trajectories under the EMPC of Eq. 38.

exists a control Lyapunov function (i.e., there exists a smooth positive-definite function V(x) that satisfies $L_fV<0$ for all states in some neighborhood of the origin when $L_{g_i}V\equiv 0$ for all $i=1,\ldots,n_u$), see, for example, Ref. 40 *for more discussion of this point. Furthermore, there exists a stabilizing controller which satisfies the conditions of Eq.* 33a–33c. *Thus, an explicit characterization of the stabilizing controller for each of the simulated control structure configurations is not given. Also, it is important to point out the EMPC is able to maintain operation in a bounded region around the economically optimal steady-state (verified by extensive simulations). Although the optimal steady-state is open-loop asymptotically stable, the main objective of applying feedback control is to maintain robustness of the operation and to optimize the process economics in a manner that cannot be achieved through open-loop operation.*

The purpose of applying EMPC to the process is to maximize the economic cost function of Eq. 36 through dynamic (off steady-state) operation of the process. First, we demonstrate that dynamic operation of the process with the cost function of Eq. 7a and constraint of Eq. 37 is better than operation at the economically optimal steady-state. In this set of simulations, control actions for all possible inputs are computed by EMPC. We apply the EMPC with the following formulation to the process

$$\begin{aligned}&\max_{u\in S(\Delta,N)}\int_0^{\tau_N} l_e(\tilde{x}(t),u(t))dt\\&\text{s.t. } \dot{\tilde{x}}(t)=f(\tilde{x}(t))+\sum_{j=1}^{4}g_j(\tilde{x}(t))u_j(t)\\&\tilde{x}(0)=x(\tau_k)\\&u(t)\in U, \forall t\in[0,\tau_N)\\&\frac{1}{\tau_M}\int_0^{\tau_M}F_{j0}C_{Aj0}\,dt=\dot{M}_{Aj0,\text{avg}}\,,\ j=1,2\end{aligned}\tag{38}$$

where the dynamic model is that of Eq. 35, the prediction horizon is $N=5$, the sampling period is $\Delta=0.05$ h, and the number of sampling periods in the operating window that the average constraint is enforced is $M=11$ (i.e., $\tau_M=0.55$ h). To numerically integrate the dynamic model, explicit Euler method is used with an integration time step of 1.0×10^{-3}h. Ipopt[41] was used to solve the nonlinear optimization problem of Eq. 38. All simulations below were completed on a desktop PC with an Intel Core® 2 Duo™ processor running an Ubuntu operating system.

The EMPC of Eq. 38 is applied to the chemical process of Eq. 35. The chemical process is initialized at a transient initial condition (i.e., off steady-state initial condition) and a length of operation of 33.0 h was simulated. The closed-loop state and input trajectories over the time period 31.0 to 33.0 h are shown in Figures 3 and 4 to illustrate the asymptotic operating behavior of the process under EMPC. The EMPC dictates a dynamic operation policy (Figures 3 and 4) through continuous manipulation of the inlet reactant concentration. However, for the heat rate inputs, the EMPC computes a constant input profile which corresponds to 100 MJ h^{-1} (i.e., the maximum allowable heat rate). The reason for this behavior is because the reaction rate is maximized at large temperature and thus, the molar flow rate of the desired product leaving the process is the largest when the maximum amount of heat is provided to the reactors. To show that the operating policy is economically better than steady-state operation, the average economic cost is defined as

$$\bar{J}_e=\frac{1}{t_f}\int_0^{t_f} l_e(x(t),u(t))dt.\tag{39}$$

For the process of Eq. 35 under EMPC, the asymptotic performance (i.e., the average economic cost after a sufficiently long operating time such that the effect of the initial condition becomes negligible) is 29.98. The economically optimal steady-state has an (average) economic cost of 28.21. Thus, asymptotic operation under EMPC is 6.27% better than steady-state operation.

Since there is a benefit in terms of the economic cost to operate the chemical process of Eq. 35 under EMPC, input selection for EMPC is considered. First, the input selection methodology (Figure 2) is applied to the chemical process example. Subsequently, closed-loop simulation results are provided to confirm this is the proper choice of input selection for EMPC. Two sets of simulations are considered. In the first set of simulations, all the possible 16 combinations of input selections for EMPC are simulated under nominal operation. In the second set, operation with process noise is considered.

Applying the input selection methodology for EMPC (Figure 2), the relative degree of the economic cost with respect to each input is computed with the directed graph method[22] (Figure 5). Based on this analysis, the inputs Q_1 and C_{A10} have a relative degree of 3, while the inputs Q_2 and C_{A20} have a relative degree of 2. No inputs have an infinite relative

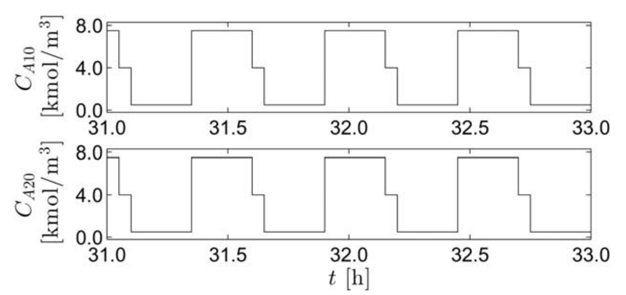

Figure 4. The manipulated input trajectories under the EMPC of Eq. 38.

The input trajectories $Q_1(t)$ and $Q_2(t)$ are not shown because they are constant profiles with $Q_i(t)=100$ MJ h^{-1}, i=1,2 over the entire 33.0 h length of operation.

degree. The normalized dynamic and steady-state sensitivities are computed. All the inputs are scaled such that $u_j \in [-1, 1]$, j=1, 2, 3, 4 and the following notation is adopted for the inputs: $u_1=(Q_1-Q_{\text{shift}})/Q_{\text{ref}}$, $u_2=(Q_2-Q_{\text{shift}})/Q_{\text{ref}}$, $u_3=(C_{A10}-C_{\text{shift}})/C_{\text{ref}}$ and $u_4=(C_{A20}-C_{\text{shift}})/C_{\text{ref}}$ where Q_{ref} and C_{ref} are scaling factors, Q_{shift} and C_{shift} are shifting constants, and the vector fields $g_1(x), g_2(x), g_3(x)$, and $g_4(x)$ are the vector fields corresponding to the inputs u_1, u_2, u_3, and u_4, respectively, from the dynamic model of Eq. 35.

The dynamic sensitivities of Eq. 24 for the inputs with relative degree of 2 are

$$S_{2,1}=L_{g_2}L_f l_{e,x}(x)=\frac{Q_{\text{ref}}\,k_0E(F_{10}+F_{20})}{\rho C_p V_2 \text{RT}_2^2}e^{-E/\text{RT}_2}C_{A2}^2 \qquad (40)$$

$$S_{2,2}=L_{g_4}L_f l_{e,x}(x)=\frac{2F_{20}C_{\text{ref}}\,k_0(F_{10}+F_{20})}{V_2}e^{-E/\text{RT}_2}C_{A2} \qquad (41)$$

for u_2 and u_4, respectively. The dynamic sensitivities are computed from the closed-loop state trajectory under the EMPC with control actions computed by EMPC for all inputs and are shown in Figure 6. The average normalized dynamic sensitivities over the length of operation are $\bar{S}_{2,1}=0.02$ and $\bar{S}_{2,2}=0.98$. From this analysis, the input u_4 has a much greater dynamic sensitivity on the economic cost than u_2. A similar analysis is completed for inputs with relative degree of 3 and their dynamic sensitivities are given by

$$S_{3,1}=L_{g_1}L_f^2 l_{e,x}(x)=\frac{Q_{\text{ref}}\,F_{10}k_0E(F_{10}+F_{20})}{\rho C_p V_1 V_2 R}\times\left(\frac{1}{T_1^2}e^{-E/\text{RT}_1}C_{A1}^2+\frac{1}{T_2^2}e^{-E/\text{RT}_2}C_{A2}^2\right) \qquad (42)$$

$$S_{3,2}=L_{g_3}L_f^2 l_{e,x}(x)=\frac{2F_{10}^2C_{\text{ref}}\,k_0F_3}{V_1V_2}\times\left(e^{-E/\text{RT}_1}C_{A1}+e^{-E/\text{RT}_2}C_{A2}\right) \qquad (43)$$

for u_1 and u_3, respectively and are shown in Figure 7. The average normalized dynamic sensitivities are $\bar{S}_{3,1}=0.01$ and $\bar{S}_{3,2}=0.99$. A similar relationship is observed, that is, the inlet concentration input u_3 has a greater dynamic sensitivity than the heat rate input u_1.

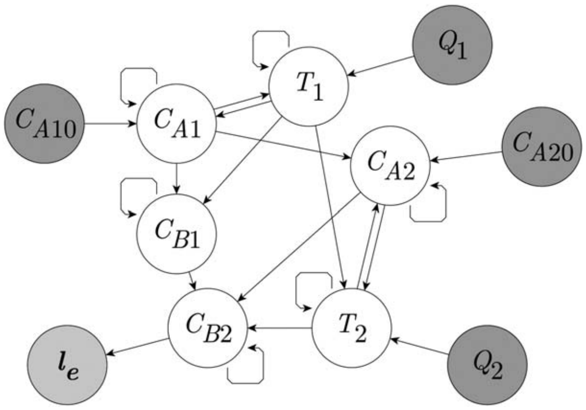

Figure 5. A directed graph constructed for the chemical process example for the economic cost function of Eq. 36 to compute the relative degree of various input variables using the methodology of Ref. 22.

The candidate manipulated inputs are dark gray and the economic cost is light gray.

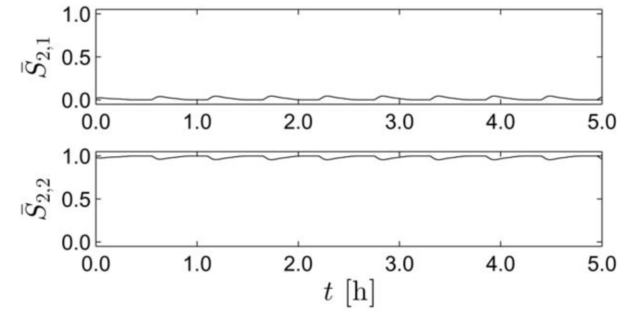

Figure 6. The dynamic sensitivities for inputs with relative degree 2 which are computed with the closed-loop state trajectory under the EMPC with all inputs on EMPC.

The dynamic sensitivity analysis identified that the inlet concentration inputs have a more substantial dynamic sensitivity compared to the heat rate inputs (comparing inputs with the same relative degree). Using steady-state sensitivity, all inputs are compared to see if these effects are significant across the set of all the possible inputs. For simplicity, the steady-state sensitivities (Eq. 32) are computed with the economically optimal steady-state and are given by

$$\begin{aligned}\hat{S}_1&=0.01\\ \hat{S}_2&=0.01\\ \hat{S}_3&=0.56\\ \hat{S}_4&=0.43\end{aligned} \qquad (44)$$

for the inputs u_1, u_2, u_3, and u_4, respectively. Based on both sensitivity analyses, the inlet concentration inputs should be placed on EMPC. Based on the relative degree analysis, Q_2 may also be placed on EMPC. However, the sensitivity analysis revealed that the economic cost is not sensitive to this input.

All 16 possible input selection combinations for EMPC are simulated. If the control action is not computed by EMPC, then it is fixed to its economically optimal steady-state value. The case where no inputs are placed on EMPC is also considered. The resulting EMPC schemes were applied to the process under nominal operation. The average economic cost for each of these cases depended only on whether C_{A10} and C_{A20} were on EMPC. If none of inlet concentrations were on EMPC, the average economic cost was $\bar{J}_e=28.22$; if C_{A10} was manipulated by EMPC and C_{A20} was

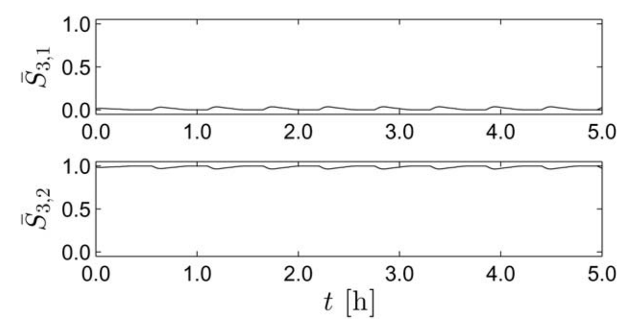

Figure 7. The dynamic sensitivities for inputs with relative degree 3 which are computed with the closed-loop state trajectory under the EMPC with all inputs on EMPC.

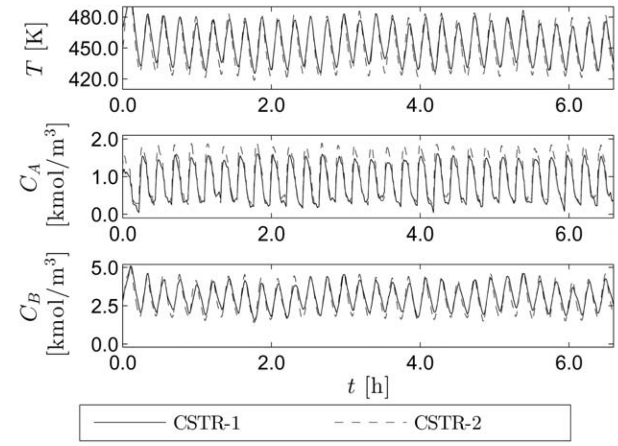

Figure 8. The closed-loop state trajectories of the chemical process under EMPC with added process noise.

fixed, the cost was $\bar{J}_e=28.54$; if C_{A10} was fixed and C_{A20} was manipulated by EMPC, the cost was $\bar{J}_e=29.57$; and if both C_{A10} and C_{A20} were on EMPC, the cost was $\bar{J}_e=30.13$. The reason the economic cost function is not influenced by the heat rates is the computed heat rate trajectories by EMPC are constant trajectories; that is, the constant trajectory when the heat rate was fixed to its economically optimal value is the same as the computed heat rate trajectory of EMPC.

From the average economic cost results, the inlet concentration C_{A20} has more of an impact on the average cost than the inlet concentration C_{A10} (the case that C_{A20} is on EMPC and C_{A10} is not on EMPC the performance is 1.1% better than the case that C_{A10} is on EMPC and C_{A20} is not on EMPC). This agrees with the relative degree of the economic cost function with respect to C_{A10} and C_{A20} which are 3 and 2, respectively. The average computation time required to solve the EMPC problem, a key metric considered in the last set of simulations, was also considered for each of the 16 simulations considered here. It was found that the computation time was mainly a function of the number of inputs whose control action was computed by EMPC (i.e., the computation time scaled with the number of decision variables) and the computation time of each EMPC with the same number of inputs were all comparable. The average computation time required to solve the EMPC with the inputs C_{A10} and C_{A20} was 36.4 ms, while, that of the EMPC with all inputs was 163.6 ms.

In the last set of simulations, process operation in the presence of process noise was considered. The process noise was modeled as bounded Gaussian noise. The process noise added to the temperature differential equations was $w_T \sim \mathcal{N}(0, 15^2)$ and was bounded by $w_{b,T}=40.0$ (i.e., $|w_T(t)| \leq w_{b,T}$); the process noise added to the concentration differential equations was $w_C \sim \mathcal{N}(0, 2^2)$ with a bound of $w_{b,C}=5.0$. The process noise was realized by generating a new random number and adding it to the right-hand side of the process model of Eq. 35 over the sampling period. Four cases were considered: (1) all the inputs were controlled by EMPC, (2) the inputs having relative degree 2 (C_{A20} and Q_2) were controlled by EMPC, (3) the inputs having relative degree 3 (C_{A10} and Q_1) were controlled by EMPC, and (4) the inputs C_{A10} and C_{A20} were controlled by EMPC. For each of the four cases, the process was initialized with the same initial condition and simulated for 16.5 h length of operation with the same realization of the process noise. The closed-loop trajectories are given in Figures 8 and 9 for the case where control actions for all inputs are computed by EMPC.

The average economic costs over the simulation for these cases were: (1) $\bar{J}_e=29.87$, (2) $\bar{J}_e=29.21$ (a decrease of 2.2% over all inputs on EMPC), (3) $\bar{J}_e=28.26$ (a decrease of 5.4% over all inputs on EMPC), and (4) $\bar{J}_e=29.87$, respectively, for each case. Furthermore, the average computation time required to solve the EMPC for each case was (1) 4041 ms, (2) 239 ms, (3) 584 ms, and (4) 718 ms, respectively. The computation time reduction going from all four inputs to two inputs was an order of magnitude as the number of decision variables in the optimization problem is a dominant factor in the computational burden of solving the optimization problem. Also, case (4) has two average constraints imposed in the optimization problem compared to cases (2) and (3) which only have one average constraint. It is important to emphasize that the same program and computer processing power were used in all cases. Thus, the comparison of the computation time is consistent. The average computation time was computed for a simulation with 320 sampling periods (i.e., the EMPC was solved 320 times). The computation time required to solve the EMPC that computes control actions for C_{A20} and Q_2 is less than the computation time of EMPC that computes control actions for C_{A10} and Q_1 (the reduction in computation time is approximately a factor of two) which suggests that the computational burden is associated with how direct is the dynamic effect of the input on the economic cost.

This example is relatively small and, thus, it may be computationally viable to compute control actions for the full set of manipulated inputs with EMPC. In the final input selection, we propose to use C_{A10} and C_{A20} as the inputs that are controlled by EMPC. The inlet concentrations are the inputs that are continuously manipulated by the EMPC which leads to dynamic operation of the process that is economically better compared to steady-state operation. The input C_{A20} has more of an impact on the closed-loop performance compared to the input C_{A10}. Even though the relative degree of the economic cost with respect to Q_2 is 2, it is not included on

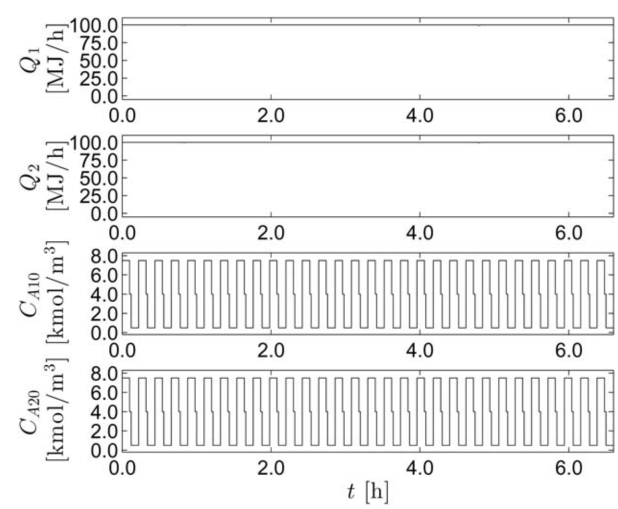

Figure 9. The manipulated input trajectories of the chemical process under EMPC with added process noise.

EMPC because practically no benefit is realized with this input on EMPC which the sensitivity analysis showed.

Conclusions

In this work, control configuration selection for EMPC was considered. A methodology to identify the manipulated inputs from the set of all possible manipulated inputs for which EMPC should compute control actions was proposed on the basis of the process economics. Since EMPC will typically enforce a dynamic operating policy, the relative degree and the sensitivities of the economic cost function with respect to an input were used to explicitly account for the nonlinear process dynamics and choose the manipulated inputs assigned to EMPC. The set of inputs selected for EMPC is guaranteed to be a stabilizing one. The overall methodology was demonstrated with a chemical process example.

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