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Contents

Economic Model Predictive Control: Handling Valve Actuator Dynamics and Process Equipment Considerations

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ABSTRACT

Chemical process equipment (e.g., sensors, valves, pumps, and vessels) can impact the dynamics, profitability, and safety of plant operation. While continuous chemical processes are typically operated at steady-state, a new control strategy in the literature termed economic model predictive control (EMPC) moves process operation away from the steady-state paradigm toward a potentially time-varying operating strategy to improve process profitability. The EMPC literature is replete with evidence that this new paradigm may enhance process profits when a model of the chemical process provides a sufficiently accurate representation of the process dynamics. Recent work in the EMPC literature has indicated that though the dynamics associated with equipment are often neglected when modeling a chemical process, they can significantly impact the effectiveness

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of an EMPC (and the potentially time-varying operating policies dictated by an EMPC may impact equipment in ways that have not been previously observed under steady-state operating policies); therefore, equipment dynamics must be accounted for within the design of an EMPC. This monograph analyzes the work that has accounted for valve behavior in EMPC to date to develop insights into the manner in which equipment behavior should impact the design process for EMPC and to provide a perspective on a number of open research topics in this direction.

Keywords: valve stiction, valve nonlinearities, economic model predictive control, process control, process safety, process equipment

1

Introduction

The limitations of process equipment (e.g., catalysts, valves, pumps, compressors, heat exchangers, vessels, and sensors), and the manner in which the materials that comprise such equipment change over time, have long been understood to pose issues for chemical process control and therefore have been accounted for in various ways. In the commonly utilized optimization-based controller known as model predictive control (MPC) (Qin and Badgwell, 2003), valve limitations are often accounted for within the control design by setting bounds on the manipulated inputs as constraints (Rawlings, 2000). Issues associated with sensors (e.g., drift and bias) have been accounted for in process control utilizing techniques such as measurement replacement (Kettunen *et al.*, 2008) and output compensation (Prakash *et al.*, 2002). Actuator faults (Venkatasubramanian *et al.*, 2003; Gajjar and Palazoglu, 2016) have been handled through reconfiguration of MPC designs (Mhaskar, 2006; Alanqar *et al.*, 2017c; Lao *et al.*, 2013). Because such equipment limitations have been recognized to play an important role in the effectiveness of MPC designs and in maintaining closed-loop stability and process operational safety, developments in economic model predictive control (EMPC) (Ellis *et al.*, 2014a; Rawlings *et al.*, 2012; Müller *et al.*, 2015; Amrit *et al.*, 2013; Limon *et al.*, 2014), which is an MPC with a modified objective function (compared to the traditional industrial design) that does not take its minimum at a process steady-state and therefore may operate a process in a time-varying fashion, can incorporate similar techniques. The methods for accounting for equipment limitations just described are handled at the design stage of MPC/EMPC when it is still possible to add appropriate constraints and abilities for model updating or controller reconfiguration to the control system.

Despite recognition of the importance of accounting for equipment limitations like hard bounds and equipment failure in MPC and EMPC, little emphasis has been placed on accounting for equipment behavior in a dynamic context. Though it could be argued that the traditional methods utilized for model updating in MPC based on process data (Marlin and Hrymak, 1996) and data-based on-line model update methods for EMPC (Alanqar *et al.*, 2017b) can account for time-varying process dynamics attributable to equipment issues such as catalyst deactivation and heat exchanger fouling, these methods do not explicitly analyze the dynamic behavior of equipment to understand how it may, like other limitations/failure mechanisms of equipment, imply that adjustment may need to be made to MPC/EMPC designs at the design stage. Several works on MPC accounting for valve behavior through various constraints (e.g., Zabiri and Samyudia, 2006; del Carmen Rodríguez Liñán and Heath, 2012) have appeared. However, these have not taken the dynamic behavior of the valves explicitly into account in the dynamic model utilized for making state predictions. Srinivasan and Rengaswamy (2008) explored a compensation method for valve stiction in which a compensating signal to be added to the output of a linear controller for a process is computed by an optimization problem with a model that includes a data-driven stiction model (it is EMPC-like, taking advantage of a prediction horizon to compute a number of compensating signals throughout this horizon and only applying the first). Several recent works (e.g., Durand *et al.*, 2017; Durand and Christofides, 2016; Bacci di Capaci *et al.*, 2017) have focused on explicitly accounting for the dynamic behavior of valves in MPC/EMPC. It has been demonstrated that in addition to updates to the model utilized for making state predictions in MPC/EMPC to handle the valve behavior, adjustments may also need to be made to the design itself, incorporating different constraints than in the case that the valve dynamics can be neglected. Furthermore, the time-varying nature of the input trajectories that may be set up under an EMPC may cause equipment considerations to become relevant that may not have been previously observed when steady-state tracking was the operational goal.

Motivated by these recent developments indicating that accounting for dynamic valve behavior in control design can be critical to the success of an MPC/EMPC formulation, we focus in this work on analyzing the literature related to valve behavior in EMPC to bring to the forefront the notion that despite the general trend in the literature toward neglecting equipment behavior, equipment behavior should be accounted for within EMPC at the design stage. Using the literature focused on accounting for valve behavior in EMPC as a guide, we highlight the necessity of accounting for equipment behavior in EMPC from an economics and a constraint satisfaction viewpoint and also indicate that it may not be possible to develop EMPCs without accounting for equipment behavior and then expect that all results will readily translate to the case with equipment behavior accounted for in the model utilized for making state predictions. To demonstrate this, we select several recent EMPC developments which have not explicitly considered process-valve or process-equipment systems within the design, and suggest that the relevant dynamics of process-equipment systems may not fit within the traditional set of assumptions developed when equipment behavior is neglected. Therefore, equipment behavior must be considered from the start of EMPC design; if it is not, it may be necessary to assess whether developments in the literature can be directly applied to practical systems in which equipment plays a role before utilizing such designs.

2

Preliminaries

2.1 Notation

The symbol $|\cdot|$ represents the Euclidean norm of a vector. The symbol $S(\Delta)$ represents the set of piecewise-defined vector functions with period Δ. The notation $t_k = t_0 + k\Delta$, $k = 0, 1, \ldots$, represents a sampling time, where t_0 ($k = 0$) is the first sampling time, and Δ is the sampling period. A scalar-valued function $V_q(\cdot)$ is positive definite if $V_q(q) > 0$ for $q \neq 0$ and $V_q(0) = 0$. A level set of V_q is denoted by $\Omega_{\rho_q} := \{q \in R^n : V_q(q) \leq \rho_q\}$. A class $\mathcal{K}$ function $\alpha : [0, a) \rightarrow [0, \infty)$ is continuous, strictly increasing, and $\alpha(0) = 0$. The notation '/' signifies set subtraction, i.e., $q \in A/B$ refers to the set $\{q \in R^n : q \in A,\ q \notin B\}$. The notation q^T denotes the transpose of a vector q.

2.2 Class of systems

In this tutorial, unless otherwise stated, we consider the following class of nonlinear continuous-time systems, which can model many chemical process systems of interest:

$$\dot{q} = f(q, u_m, w), \tag{2.1}$$

where $q \in Q \subseteq R^n$ is the vector of states bounded within the set Q, $u_m \in R^m$ is the vector of control actions, and $w \in R^l$ is a vector of time-varying, bounded disturbances ($w \in W := \{w \in R^l : |w| \leq \theta\}$). In general, it is not required that u_m be equal to the vector of process inputs u_a, which may be related to the vector of process states through a nonlinear relationship (i.e., u_a can be a function of the states affected by u_m, rather than a manipulated input). Physically, the process inputs are outputs from final control elements (e.g., flow rates out of valves, heat inputs from heating coils) that are subject to actuator limitations and hence u_a is assumed to be bounded (i.e., $u_a \in U_a := \{u_a \in R^m : u_{a,i}^{\min} \leq u_{a,i} \leq u_{a,i}^{\max},\ i = 1, \ldots, m\}$), where $u_{a,i}$ represents the i-th component of u_a and $u_{a,i}^{\min}$ and $u_{a,i}^{\max}$ are its lower and upper bounds, respectively. The components of the vector u_m may correspond to different quantities than u_a corresponds to (for example, they may be control signals or set-points sent to valve actuators). However, due to the relationship with the process inputs, they should also be bounded (i.e., $u_m \in U_m$). When dynamics related to process equipment can be neglected (e.g., when the valve dynamics are significantly faster than the process dynamics), Equation (2.1) provides a reasonably accurate model of the system behavior with q containing only the process states, and u_a and u_m can be assumed to be equivalent. In general, however, q can include states related to both the process and the equipment states, and static or dynamic equations may relate u_a and u_m. For simplicity of notation in this monograph, we will use the short-hand notation $f(q, u_m)$ to designate the process of Equation (2.1) in the absence of disturbances (i.e., $w(t) \equiv 0$), which will be referred to as the nominal model.

Though the discrete-time counterpart of Equation (2.1) is considered in many works on EMPC (e.g., Amrit *et al.*, 2011; Diehl *et al.*, 2011; Rawlings *et al.*, 2012), this work will discuss continuous-time systems due to the fact that they arise naturally in the first-principles modeling of chemical processes. The results discussed could be examined for extension to EMPC for discrete-time systems (Alessandretti *et al.*, 2016).

2.3 Economic model predictive control

Economic model predictive control (EMPC) is a model-based control design that determines appropriate control actions for a process by solving the following optimization problem:

$$\min_{u_m(t)\in S(\Delta)} \quad \int_{t_k}^{t_{k+N}} L_e(\tilde{q}(\tau), u_m(\tau))\, d\tau \tag{2.2a}$$

$$\text{s.t.} \quad \dot{\tilde{q}}(t) = f(\tilde{q}(t), u_m(t)) \tag{2.2b}$$

$$\tilde{q}(t_k) = q(t_k) \tag{2.2c}$$

$$\tilde{q}(t) \in Q,\ \forall\, t \in [t_k, t_{k+N}) \tag{2.2d}$$

$$u_m(t) \in U_m,\ \ \forall\, t \in [t_k, t_{k+N}) \tag{2.2e}$$

where the stage cost L_e is optimized over a prediction horizon consisting of N sampling periods of length Δ (throughout each sampling period, a constant value of u_m is computed, which is reflected by the notation $u_m(t) \in S(\Delta)$ in Equation (2.2a). The notation $\tilde{q}$ signifies the prediction of the state q from the nominal model in Equation (2.2b) from the initial condition in Equation (2.2c) which corresponds to a state measurement at time t_k. Equations (2.2d)–(2.2e) reflect state and input constraints, respectively (Equation (2.2d) may include bounds on states related to u_a, since if $u_a \neq u_m$, the bound in Equation (2.2e) does not necessarily prevent valve output saturation). The stage cost in Equation (2.2a) is not required to take its minimum at a process steady-state, as is required in the traditional tracking MPC designs utilized in industry. However, tracking MPC is a special case of EMPC (it is an EMPC with a quadratic objective function), and therefore the results in this work should be understood to be applicable to MPC.

3

Handling Process-Equipment Considerations within EMPC

Under the assumption that $u_a = u_m$, a variety of modifications have been made to Equation (2.2) (e.g., various constraints or restrictions on the horizon length, process model, and/or objective function have been added; reviews of formulations of various EMPC designs developed to guarantee closed-loop stability and feasibility can be found in Ellis *et al.*, 2014a; Ellis *et al.*, 2016; Rawlings *et al.*, 2012; Müller and Allgöwer, 2017) to address theoretical (e.g., closed-loop stability) and practical (e.g., operational safety, Albalawi *et al.*, 2017c) considerations. From the generality of the process model incorporated in Equation (2.2) and its modifications, it may be supposed that new EMPC developments in the literature should be able to be readily applied to a chemical process system in which equipment dynamics are not negligible simply by using an appropriate dynamic model in Equation (2.2b) that explicitly includes dynamics related to equipment. A goal of this section is to demonstrate that based on recent results in the literature that seek to explicitly handle valve considerations within EMPC, a comparison with several example formulations that do not, and an analysis of potential limitations of other types of dynamics related to equipment, this may not be the case.

3.1 EMPC accounting for valve behavior

Several recent works (Durand *et al.*, 2014; Durand and Christofides, 2016; Durand *et al.*, 2017) have explicitly examined the implications of including the valve dynamics (which cause u_a not to equal u_m) in Equation (2.2b) in addition to the dynamics of the chemical process. This acknowledges that the controller, process, and valve dynamics are coupled (i.e., the equipment is not independent of the process) so that an EMPC made aware of the valve dynamics can make better choices for control actions because it is using a more accurate process model. Though this is an example of the well-known principle that MPCs/EMPCs compute more optimal input trajectories when a more accurate model is utilized for making state predictions, it is conceptually different from what is commonly implied by this principle. Specifically, this principle typically is applied with respect to improving the model of the chemical process, not with recognizing how commonly neglected dynamics such as those of equipment are playing a role in the accuracy of the dynamic model.

Valve dynamics vary between valves, and are influenced by a variety of factors, such as the type of the valve (e.g., butterfly, globe, ball; Bishop *et al.*, 2002), the mechanism by which the valve moves, the lubrication of the valve, and the types of effects that cause $u_a \neq u_m$ (e.g., a valve may exhibit nonlinear dynamic behavior associated with friction called stiction or may experience delays in changes in its output termed backlash related to looseness of mechanical components in the valve Choudhury *et al.*, 2005). Furthermore, a valve's dynamics can change over time as a result of factors such as wear, vibration, or tightening of valve packing (Hägglund, 2002). In addition, the dynamics between $u_{a,i}$ (the i-th component of u_a) and $u_{m,i}$ (the i-th component of u_m) can be influenced by the presence of flow controllers for valves in the control loop. These might be attractive for a process under a controller like EMPC that determines $u_{m,i}$ and applies it for a sampling period. A flow controller may aid in driving $u_{a,i}$ to $u_{m,i}$ at a reasonable rate during the sampling period throughout which the set-point is fixed (Figure 3.1). Therefore, the model utilized in Equation (2.2b) (which can be either a first-principles or empirical model of valve behavior;

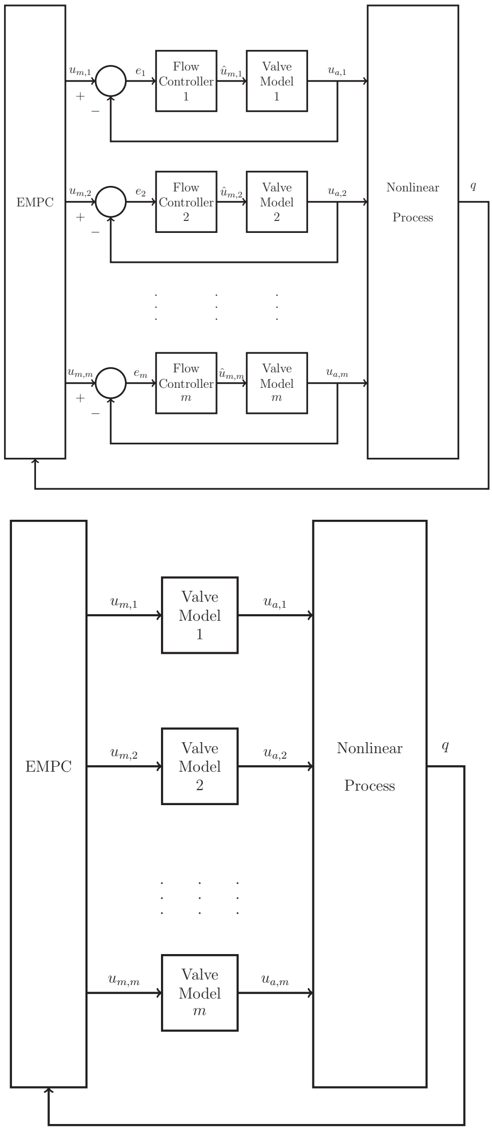


Figure 3.1: Schematic portraying potential configurations of the EMPC output u_m and the valve output vector u_a. The top figure shows the control architecture in the case that the valve output flow rate set-points $u_{m,i}$, $i = 1, \ldots, m$, from the EMPC are set-points for a flow controller for a valve. e_i and $\hat{u}_{m,i}$, $i = 1, \ldots, m$, denote the error $u_{m,i} - u_{a,i}$ received by the flow controller and the flow controller output, respectively. The bottom figure portrays the control loop architecture when no valves are operated under flow control. In both figures, q represents measurements of states for the process-valve system that the EMPC receives as state feedback.

see Brásio *et al.*, 2014, for example, for a review of many modeling techniques for friction in valves, and Durand *et al.*, 2017 for an example of an empirical model of a sticky valve's flow controller and dynamics developed for use in EMPC) will need to take into account the individual nature of the dynamics of each valve influencing the process.

To exemplify how valve dynamics may be cast in a nonlinear systems framework, we discuss very general forms for two classes of valve dynamics. The first, which was investigated in (Durand *et al.*, 2014), describes the case that a linear relationship relates $u_{a,i}$ to $u_{m,i}$, as follows:

$$\begin{aligned} \begin{bmatrix} \dot{x}_{a,i}(t) \\ \dot{\zeta}_i(t) \end{bmatrix} &= A_i \begin{bmatrix} x_{a,i}(t) \\ \zeta_i(t) \end{bmatrix} + B_i u_{m,i}(t) \\ u_{a,i}(t) &= C_i x_{a,i}(t) \end{aligned} \tag{3.1}$$

where $x_{a,i} \in R^{n_{s_i}}$, $i = 1, \ldots, m$ is a vector of $n_{s,i}$ states describing the dynamics of the i-th valve, and $\zeta_i \in R^{n_{c,i}}$, $i = 1, \ldots, m$, is a vector of $n_{c,i}$ dynamic states of a linear flow controller, and $A_i \in R^{(n_{s,i}+n_{c,i})\times(n_{s,i}+n_{c,i})}$, $B_i \in R^{(n_{s,i}+n_{c,i})\times 1}$, and $C_i \in R^{1\times n_{s,i}}$ are matrices and vectors.

Nonlinear models of valve behavior may also be required (e.g., when a valve experiences stiction). In that case, the $u_{a,i} - u_{m,i}$ relationship may be characterized through nonlinear systems of differential equations as follows:

$$u_{a,i} = f_{a,i}(x_{dyn,i}) \tag{3.2}$$

$$\dot{x}_{dyn,i} = f_{dyn,i}(x_{dyn,i}, u_{m,i}), \tag{3.3}$$

where $x_{dyn,i} \in R^{n_{z_i}}$ is a vector of states describing the dynamics related to the i-th valve (including those related to a flow controller for a specific valve if applicable), and $f_{a,i}$ and $f_{dyn,i}$ are nonlinear functions (scalar-valued and vector-valued, respectively) describing the relationship between $u_{a,i}$ and $x_{dyn,i}$ and $u_{m,i}$. In the notation of Equation (2.1), q includes all states associated with the process (components of the vector x) and with the valve, i.e., $q = [x\ x_{dyn}]^T$, where $x_{dyn} = [x_{dyn,1}\ \ldots\ x_{dyn,m}]^T$.

To provide more context to the modeling in Equations (3.2)–(3.3), consider that one way of obtaining a first-principles model for a valve experiencing stiction is to perform a force balance on the valve and select an appropriate model of the friction dynamics to model the friction force in this force balance. If the LuGre model Canudas de Wit *et al.* (1995) is selected as this friction model and the valve is modeled as a pneumatic sliding-stem globe valve such that the forces on the valve can be modeled as being due to the friction force, spring force, and pressure from the pneumatic actuation (Choudhury *et al.*, 2005), the valve dynamics may be modeled through the following dynamic equations (which take the form of Equation (3.3)):

$$\frac{dx_v}{dt} = v_v \tag{3.4}$$

$$\frac{dv_v}{dt} = \frac{1}{m_v}\left[A_v P - k_s x_v - \sigma_0 z_f - \sigma_1 v_v \right.$$
$$\left. + \frac{\sigma_1 |v_v| \sigma_0 z_f}{F_C + (F_S - F_C)e^{-(v_v/v_s)^2}} - \sigma_2 v_v\right] \tag{3.5}$$

$$\frac{dz_f}{dt} = v_v - \frac{|v_v|\sigma_0 z_f}{F_C + (F_S - F_C)e^{-(v_v/v_s)^2}}, \tag{3.6}$$

where x_v is the valve stem position, $x_{v,\max}$ is the maximum valve stem position, $u_{a,\max}$ is the maximum flow rate through the valve, v_v is the valve velocity, k_s is the spring constant for the spring of the globe valve, A_v is the area of the valve diaphragm, P is the pressure applied to the diaphragm by the pneumatic actuation, and m_v is the mass of the valve moving parts. The state z_f is an internal state of the LuGre friction model, which is used in Equations (3.5) and (3.6) to model the friction force experienced by the valve moving parts. F_S, F_C, v_s, σ_0, σ_1, and σ_2 are parameters of this friction model. A relationship between u_a and x_v might be developed from a valve characteristic (Coughanowr and Leblanc, 2009) to relate u_a and x_v as in Equation (3.2) (an example is provided below). The value of P can be determined by a controller (i.e., it is related to u_m).

The EMPC designs from Durand *et al.* (2014) and Durand and Christofides (2016) imply that if an EMPC of the form of Equation (2.2) is developed assuming $u_a = u_m$, but it is desired to update it to reflect the valve behavior, the required updates may not be as simple as using a process-valve model in Equation (2.2b). If it is desired for the objective function, for example, to reflect that profits depend on the actual process input vector u_a rather than its set-point vector u_m, the objective function will need to reflect this. Furthermore, the potential for an EMPC to set up a time-varying operating policy may necessitate the use of constraints (termed "economic constraints") designed to prevent the controller from setting up an undesirable operating policy that might increase costs (e.g., increase feedstock costs by adjusting the manipulated inputs) that are not reflected in the objective function (an example of an economic constraint is presented below). Economic constraints may be functions of process inputs; this could result in cases where, if u_a is assumed to equal u_m, the economic constraints are functions of the manipulated inputs, but when $u_a \neq u_m$, they may instead be state constraints. Valve dynamics may also introduce a need for new state, input, or combined state and input constraints that are not present when $u_a = u_m$ (an example of this will be showcased below). This again implies that valve dynamics must be considered from the beginning of the design of EMPC formulations, because these dynamics may result in fundamentally different types and numbers of constraints than may be considered reasonable when $u_a = u_m$. This can impact not only individual formulations, but even theoretical results because changes in the type and formulation of constraints can impact how feasibility is considered for an EMPC formulation at the design stage.

Example 1. To exemplify how accounting for valve behavior may result in modifications to the model, constraints, and objective function of an EMPC, we consider controlling an ethylene oxidation process (Özgülşen *et al.*, 1992; Alfani and Carberry, 1970) with the following dynamic model written in dimensionless form:

$$\dot{x}_1 = u_a(1 - x_1 x_4) \tag{3.7a}$$

$$\dot{x}_2 = u_a(0.5 - x_2 x_4) - A_1 exp(\gamma_1/x_4)(x_2 x_4)^{0.5} - A_2 exp(\gamma_2/x_4)(x_2 x_4)^{0.25} \tag{3.7b}$$

$$\dot{x}_3 = -u_a x_3 x_4 + A_1 exp(\gamma_1/x_4)(x_2 x_4)^{0.5} - A_3 exp(\gamma_3/x_4)(x_3 x_4)^{0.5} \tag{3.7c}$$

$$\dot{x}_4 = \frac{u_a}{x_1}(1 - x_4) + \frac{B_1}{x_1} exp(\gamma_1/x_4)(x_2 x_4)^{0.5} + \frac{B_2}{x_1} exp(\gamma_2/x_4)(x_2 x_4)^{0.25} + \frac{B_3}{x_1} exp(\gamma_3/x_4)(x_3 x_4)^{0.5} - \frac{B_4}{x_1}(x_4 - 1) \tag{3.7d}$$

where $x = [x_1\ x_2\ x_3\ x_4]^T$, and x_1, x_2, x_3, and x_4 are the dimensionless gas density, ethylene concentration, ethylene oxide concentration, and reactor temperature, respectively. The single process input u_a represents the dimensionless feed volumetric flow rate, which is related to the valve output flow rate set-point u_m computed by a controller through Equations (3.4)–(3.6), with the following equations describing the valve characteristic and PI control law for the flow controller of the valve that computes the pressure applied by the pneumatic actuation, respectively:

$$u_a = \left(\frac{x_{v,\max} - x_v}{x_{v,\max}} \right) u_{a,\max} \tag{3.8}$$

$$P = P_s + K_{c,p} \frac{u_m - u_a}{u_{a,\max}} + \frac{K_{c,p}}{\tau_{I,p}} \zeta_P \tag{3.9}$$

$$\dot{\zeta}_P = \frac{u_m - u_a}{u_{a,\max}} \tag{3.10}$$

where the controller tuning is $K_{c,p} = -82737.09$ and $\tau_{I,p} = 0.01$, and P_s is a steady-state pressure value (fixed to the last applied value of the pressure whenever u_m changes). ζ_P is the dynamic state of the PI controller, and it is re-initialized to zero every time that u_m changes. The values of the parameters in these equations are noted in Table 3.1 (Garcia, 2008; Özgülşen *et al.*, 1992).

Two EMPCs will be examined for controlling this process (i.e., for computing u_m) over two operating periods of length t_p, where t_p is one dimensionless time unit (denoted by t_d; i.e., $t_p = 1\ t_d$). The prediction horizon N_k shrinks throughout an operating period (it is 5 at the beginning of the operating period, and decreases by one at each subsequent sampling time in the operating period so that the prediction horizon always includes the remainder of the operating period). A sampling period has length $\Delta = 0.2\ t_d$. The first EMPC

Table 3.1: Ethylene oxidation example parameters. t_d denotes a dimensionless time unit.

Parameter	Value
γ_1	–8.13
γ_2	–7.12
γ_3	–11.07
A_1	92.80
A_2	12.66
A_3	2412.71
B_1	7.32
B_2	10.39
B_3	2170.57
B_4	7.02
m_v	1.361 kg
A_v	0.06452 m^2
k_s	52538 kg/t_d^2
v_s	0.000254 m/t_d
σ_0	10^8 kg/t_d^2
σ_1	9000 kg/t_d
σ_2	612.9 kg/t_d
F_C	1423 $kg \cdot m/t_d^2$
F_S	1707.7 $kg \cdot m/t_d^2$
$u_{a,\max}$	0.7042
$x_{v,\max}$	0.1016 m

to be examined accounts for the valve behavior and is formulated as follows, where $q = [x^T \; x_v \; v_v \; z_f \; \zeta_P]^T$ and $\dot{q} = f_q(q, u_m)$, used in making state predictions within the controller, denotes the dynamic system of Equations (3.7), (3.4)–(3.6), and (3.8)–(3.10):

$$\min_{u_m(t) \in S(\Delta)} \quad \int_{t_k}^{t_{k+N_k}} -\tilde{u}_a(\tau)\tilde{x}_3(\tau)\tilde{x}_4(\tau)\,d\tau \tag{3.11a}$$

$$\text{s.t.} \quad \dot{\tilde{q}}(t) = f_q(\tilde{q}(t), u_m(t)) \tag{3.11b}$$

$$\tilde{q}(t_k) = q(t_k) \tag{3.11c}$$

$$0 \leq \tilde{u}_a(t) \leq 0.7042,\ \forall\, t \in [t_k, t_{k+N_k}] \tag{3.11d}$$

$$0.0704 \leq u_m(t) \leq 0.7042,\ \forall\, t \in [t_k, t_{k+N_k}] \tag{3.11e}$$

$$\tilde{P} \geq 0,\ \forall\, t \in [t_k, t_{k+N_k}) \tag{3.11f}$$

$$\int_{t_k}^{t_{k+N_k}} \tilde{u}_a(\tau)d\tau + \int_{(j-1)t_p}^{t_k} u_a^*(\tau)d\tau = 0.175t_p/0.5 \tag{3.11g}$$

In Equation (3.11), j denotes the number of complete operating periods that have passed before the current sampling period, and $\tilde{q}$ signifies the prediction of the process-valve state from Equation (3.11b). $\tilde{u}_a$ is the prediction of u_a (obtained from the predicted value of x_v from Equation (3.8)), which is bounded between the maximum and minimum flow rates considered to be achievable from the valve (Equation (3.11d)). $u_a^*(t)$ represents the actual valve output at time $t < t_k$. The objective function is related to the time-averaged yield of ethylene oxide with a fixed available feedstock. Equation (3.11g) is an example of an "economic constraint" for an EMPC, requiring that the amount of feedstock used by the process in each time interval of length t_p be fixed to 0.175, which is the amount which would be fed at steady-state. $\tilde{P}$ represents the predicted value of the pressure from the pneumatic actuation, and because pressure cannot become negative, it is required to be positive throughout the prediction horizon under any input trajectory returned by Equation (3.11). This is a constraint on both states and the manipulated input u_m, as can be seen from Equation (3.9) and the fact that ζ_P is a state of the process-valve system and that u_a is a function of a state through Equation (3.8).

The second EMPC neglects the dynamics of the valve (i.e., it assumes $u_a = u_m$) and is formulated as follows, where $\dot{x} = f_x(x, u_m)$ denotes the dynamic system of Equation (3.7) with $u_a = u_m$ and $u_m^*(t)$ denotes the value of the manipulated input applied by the EMPC at time $t < t_k$:

$$\min_{u_m(t) \in S(\Delta)} \quad \int_{t_k}^{t_{k+N_k}} -u_m(\tau)\tilde{x}_3(\tau)\tilde{x}_4(\tau)\, d\tau \tag{3.12a}$$

$$\text{s.t.} \quad \dot{\tilde{x}}(t) = f_x(\tilde{x}(t), u_m(t)) \tag{3.12b}$$

$$\tilde{x}(t_k) = x(t_k) \tag{3.12c}$$

$$0.0704 \leq u_m(t) \leq 0.7042, \forall\, t \in [t_k, t_{k+N_k}) \tag{3.12d}$$

$$\int_{t_k}^{t_{k+N_k}} u_m(\tau)d\tau + \int_{(j-1)t_p}^{t_k} u_m^*(\tau)d\tau = 0.175t_p/0.5 \tag{3.12e}$$

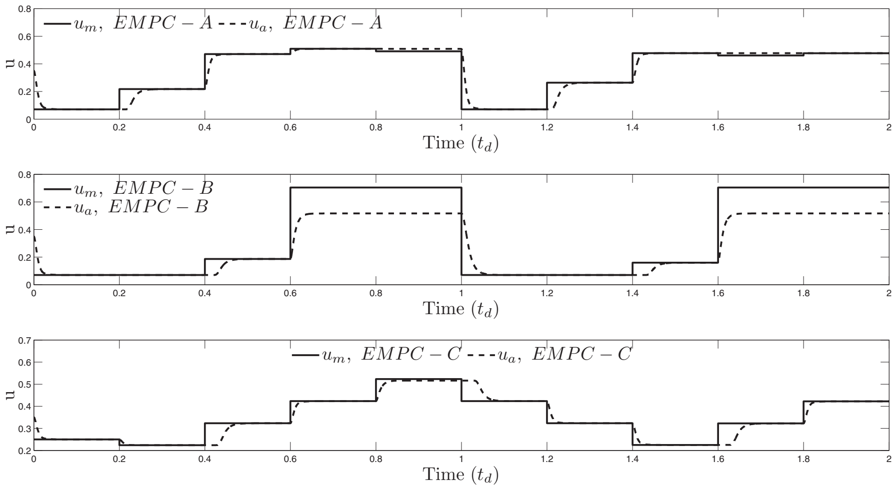
In Equation (3.12), $\tilde{x} = [\tilde{x}_1\ \tilde{x}_2\ \tilde{x}_3\ \tilde{x}_4]^T$ represents the predicted state of the system of Equation (3.7). Again, the objective function is related to the time-averaged process yield with a fixed available feedstock and the economic constraint is again related to a feedstock restriction, but here both consider that $u_a = u_m$.

The results of controlling the process of Equations (3.7), (3.4)–(3.6), and (3.8)–(3.10) with both of these EMPCs are shown in Figure 3.2, where the trajectories of u_a, u_m, and P under the first EMPC are labeled with "EMPC-A," and those under the second EMPC are labeled with "EMPC-B." The simulations were performed using Ipopt (Wächter and Biegler, 2006), with an integration step size of $10^{-6}\ t_d$ utilized within the first EMPC and an integration step size of $10^{-4}\ t_d$ utilized within the second, and the process model of Equations (3.7), (3.4)–(3.6), and (3.8)–(3.10) simulated within an integration step size of $10^{-6}\ t_d$ under the inputs computed by both EMPCs. The pressure for the pneumatic actuation of the process was saturated at zero if it would otherwise have become negative. The simulation was initiated from the process–valve state $q_I = [0.997\ 1.264\ 0.209\ 1.004\ 0.051\ m\ 2.000 \times 10^{-6}\ m/t_d\ 1.426 \times 10^{-5}\ m\ 0]^T$, with the initial value of P_s set to 63713 $kg/m \cdot t_d^2$. Further details regarding the simulation can be found in Durand and Christofides (2016). The results indicate that incorporating the valve dynamics improved the ability of the EMPC to compute set-points for which the available actuation energy was sufficient to drive the valve output flow rate to the set-point. This is important due to the economic constraint, which is satisfied under the first EMPC but not under the second EMPC because the plant-model mismatch for the second EMPC causes that control actions computed by that EMPC (which would need to be reached by u_a to ensure that the feedstock constraint is met) to not be reachable with the available pressure from the pneumatic actuation.

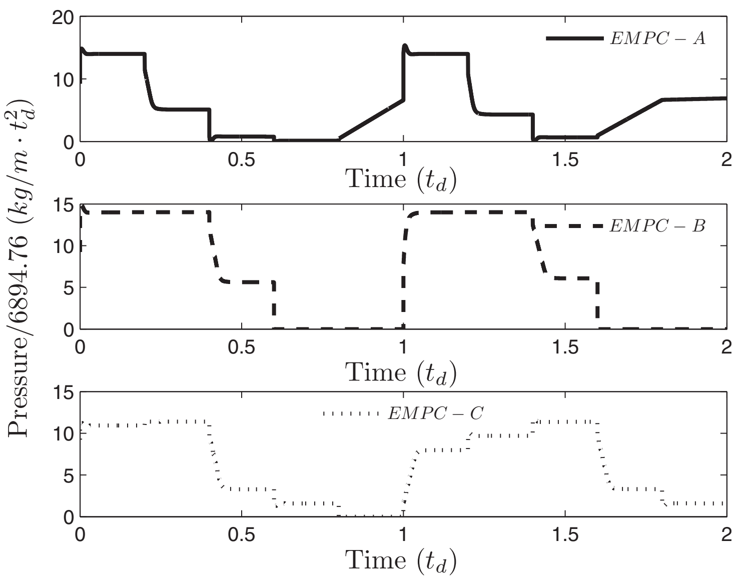
Comparing Equations (3.11) and (3.12) indicates that the objective functions of the optimization problems are formulated differently. That in Equation (3.11) is formulated with respect to u_a (as opposed to u_m as in Equation (3.12)) due to a recognition that it is the physical process inputs that affect the yield, not the set-points. The formulation of the economic constraint in Equation (3.12e) is also different from that in Equation (3.11g) because the actual feed to the process (the output from valves, rather than their set-points) determines how much of the feedstock has been used. Therefore, if it is assumed that $u_a = u_m$, the feedstock constraint can be applied to past and predicted inputs (Equation (3.12e)), but when it is recognized that $u_a \neq u_m$, this constraint is formulated with respect to past and future states (Equation (3.11g)). Finally, the actuation magnitude constraints are added in Equation (3.11f) because a dynamic relationship exists between u_a and u_m. Therefore, unless appropriate bounds on u_m are determined in light of this dynamic relationship that ensure that the range of values of u_m allowed corresponds only to the range of u_a that can be reached with positive pressures from the pneumatic actuation, an additional constraint may be needed to prevent actuator (pressure) saturation. This is an important physically-based constraint that cannot be included without accounting for the dynamics of the full process–valve system in the controller. It is noted that the EMPC formulations presented do not have any stability-based constraints, demonstrating that the conclusions of this section (i.e., accounting for equipment behavior in EMPC may not be as simple as updating the nonlinear process model of an EMPC formulation) are independent of the specific EMPC formulation under consideration.

3.1.1 EMPC accounting for valve behavior: Input rate of change constraints

In addition to constraints like the actuation magnitude constraints, input rate of change constraints (Durand *et al.*, 2016) have also been investigated for use in EMPC accounting for valve considerations. Specifically, they were considered to help prevent valve wear because an EMPC may compute a time-varying operating policy to maximize



(a) Value output flow rate set-point u_m compared with actual valve output u_a under three different EMPC's: EMPC-A (accounts for valve behavior), EMPC-B (assumes $u_a = u_m$), and EMPC-C (assumes $u_a = u_m$ but incorporates input of change constraints).



(b) Pressure from the pneumatic actuation under three different EMPC-A (accounts for valve behavior), EMPC-B (assumes $u_a = u_m$), and EMPC-C (assumes $u_a = u_m$ but incorporates input of change constraints).

Figure 3.2: u_a, u_m, and P for the process of Equations (3.7), (3.4)–(3.6), and (3.8)–(3.10) under three different EMPC designs demonstrating the effects of accounting and not accounting for valve behavior within the EMPC on the ability of u_a to reach u_m within each sampling period.

the objective function of Equation (2.2), and may change the process inputs between sampling periods significantly to do so (for example, Figure 3.2a shows several relatively large changes in u_m and u_a between two sampling periods for EMPC-A and EMPC-B). If the sampling period is small, this may correspond to frequent and significant movement of the valve, which may contribute to wear of the valve. Increasing the sampling period to avoid moving the valve excessively may not be a viable option because the sampling period needs to be small enough to ensure adequate control (i.e., the sampling period should not be greater than the timescale of the process), and shorter sampling periods also allow more frequent feedback of the process state, which may enhance robustness. Therefore, it may be desirable to add constraints of the following form to Equation (2.2) to set an explicit upper-bound $\epsilon_{desired,i} > 0$ for the i-th input on the amount by which the manipulated inputs (related to the valve outputs) can vary between two sampling periods of the prediction horizon:

$$|u^*_{m,i}(t_k|t_k) - u^*_{m,i}(t_{k-1}|t_{k-1})| \leq \epsilon_{desired,i}, \ \forall\ i = 1, \ldots, m \tag{3.13}$$

$$\begin{aligned} |u^*_{m,i}(t_j|t_k) - u^*_{m,i}(t_{j-1}|t_k)| \leq \epsilon_{desired,i}, \ \forall\ i = 1, \ldots, m, \\ j = k+1, \ldots, k+N-1, \end{aligned} \tag{3.14}$$

where $u^*_{m,i}(t_j|t_k)$, $j = k, \ldots, k+N-1$, signifies the optimal solution of an EMPC at time t_k for $t \in [t_j, t_{j+1})$ in the prediction horizon.

Tracking MPC designs have long incorporated constraints on the input rate of change and also penalties in the objective function on the input rate of change (Qin and Badgwell, 2003; Camacho and Bordons, 2007; Mhaskar and Kennedy, 2008); however, these constraints are particularly relevant to consider for EMPC for the following reasons: 1) It is possible that in a case without disturbances/plant-model mismatch, a tracking MPC with input rate of change constraints may be stabilizing in the sense that it may essentially drive the closed-loop state to the operating steady-state and maintain the state at this steady-state thereafter. In such a case, input aggressiveness is only problematic during the transient as the state is driven from an initial condition to the operating steady-state by an MPC. However, an EMPC may operate a process in a time-varying fashion over time even in the absence of disturbances, so that input aggressiveness remains problematic throughout the time of operation and an EMPC has potential in that case to cause greater wear of valves than a tracking MPC. 2) In the presence of disturbances, it cannot be determined *a priori* whether an MPC or EMPC will create greater actuator wear. This is because both utilize different objective functions and constraints, and therefore it cannot be determined *a priori* what control action each will compute at each measured state of the state trajectory under the inputs computed by each controller. 3) If a penalty on the input rate of change is added to the objective function of a tracking MPC, the minimum of the objective function remains the operating steady-state. In contrast, because the minimum value of the objective function of an EMPC may not be at a process steady-state, adding a penalty on the input rate of change to the objective function can directly impact the economic performance of the closed-loop system because then the EMPC is optimizing a trade-off between economic optimality with respect to a chosen profit metric and the input rate of change. This means that the weighting of any penalty on the input rate of change in the objective function of an EMPC must be carefully chosen to avoid reducing economic performance unnecessarily. 4) Restricting the allowable inputs for EMPC at a given sampling time using input rate of change constraints has the potential to reduce profits. Therefore, the bounds $\epsilon_{desired,i}$ on the input rate of change should be carefully chosen.

Input rate of change constraints are an example of constraints that may need to be added to an EMPC to account for valve behavior that are not necessarily straightforward to add to an existing EMPC design (and once again convey the need to account for equipment at the design stage rather than assuming that developing a more detailed process model will be sufficient to account for equipment behavior). A difficulty with input rate of change constraint design comes from the fact that these constraints restrict the allowable values of the inputs, which can impact the feasibility of an EMPC (e.g., they may make it more difficult for the controller to ensure that state constraints can be satisfied) and therefore must be designed in conjunction with the rest of the constraints to aid in maintaining feasibility. Constraints that guarantee that Equations (3.13) and (3.14) are satisfied by the control actions computed by an EMPC, but do so by adding constraints that are guaranteed to be feasible at each sampling time under certain assumptions, have appeared only for a specific formulation of EMPC known as Lyapunov-based EMPC (LEMPC) (Heidarinejad *et al.*, 2012). Describing this formulation requires the following two assumptions to be placed on the class of systems of Equation (2.1):

Assumption 1. The right-hand side of Equation (2.1) is a locally Lipschitz function of its arguments with an (isolated) equilibrium point at the origin of the nominal (i.e., $w(t) \equiv 0$) system with $u_m \equiv 0$ (i.e., $f(0, 0, 0) = 0$).

Assumption 2. There exists an explicit stabilizing Lyapunov-based controller $h_q(q)$ with $h_q(0) = 0$ and locally Lipschitz components that, when applied continuously to the nominal system of Equation (2.1) as the input u_m, can render the origin of that system asymptotically stable in the sense that there exists a sufficiently smooth positive definite Lyapunov function $V_q(q)$ and class $\mathcal{K}$ functions $\alpha_{1,q}$, $\alpha_{2,q}$, $\alpha_{3,q}$, and $\alpha_{4,q}$ for which the following properties hold for all $q \in D_q$:

$$\alpha_{1,q}(|q|) \leq V_q(q) \leq \alpha_{2,q}(|q|) \tag{3.15a}$$

$$\frac{\partial V_q(q)}{\partial q} f(q, h_q(q)) \leq -\alpha_{3,q}(|q|) \tag{3.15b}$$

$$\left| \frac{\partial V_q(q)}{\partial q} \right| \leq \alpha_{4,q}(|q|) \tag{3.15c}$$

$$h_q(q) \in U_m, \tag{3.15d}$$

where the Lyapunov level set $\Omega_{\rho_q} \subset D_q$, where $q \in Q$ for all $q \in \Omega_{\rho_q}$, is the stability region of the process-valve system, and D_q is a neighborhood of the origin.

With these assumptions and some additional sufficient conditions, the following formulation of an LEMPC with input rate of change constraints that are guaranteed to be feasible at each sampling time was developed (Durand *et al.*, 2016; Durand and Christofides, 2016):

$$\min_{u_m(t)\in S(\Delta)} \int_{t_k}^{t_{k+N}} L_e(\tilde{q}(\tau), u_m(\tau))\, d\tau \tag{3.16a}$$

$$\text{s.t.} \quad \dot{\tilde{q}}(t) = f(\tilde{q}(t), u_m(t)) \tag{3.16b}$$

$$\tilde{q}(t_k) = q(t_k) \tag{3.16c}$$

$$\tilde{q}(t) \in Q,\ \forall\, t \in [t_k, t_{k+N}) \tag{3.16d}$$

$$u_m(t) \in U_m,\ \ \forall\, t \in [t_k, t_{k+N}) \tag{3.16e}$$

$$V_q(\tilde{q}(t)) \le \rho_{q,e},\ \ \forall\ t \in [t_k, t_{k+N}),\ \text{ if } V_q(q(t_k)) \le \rho_{q,e} \tag{3.16f}$$

$$\frac{\partial V_q(q(t_k))}{\partial q} f(q(t_k), u_m(t_k)) \le \frac{\partial V_q(q(t_k))}{\partial q} f(q(t_k), h_q(q(t_k))),$$
$$\text{if } t_k > t_s \text{ or } V_q(q(t_k)) > \rho_{q,e} \tag{3.16g}$$

$$|u_{m,i}(t_k) - h_{q,i}(q(t_k))| \le \epsilon_{r,i},\ \ \forall\ i = 1, \ldots, m \tag{3.16h}$$

$$|u_{m,i}(t_j) - h_{q,i}(\tilde{q}(t_j))| \le \epsilon_{r,i},\ \ \forall\ i = 1, \ldots, m,$$
$$j = k+1, \ldots, k+N-1, \tag{3.16i}$$

where t_s is the time after which Equation (3.16g) begins to be enforced regardless of the value of $V_q(q(t_k))$, and $\epsilon_{r,i}$ is an upper bound in Equations (3.16h)–(3.16i) ($\epsilon_{r,i} \neq \epsilon_{desired,i}$). $\Omega_{\rho_{q,e}} \subset \Omega_{\rho_q}$ defines a region in state-space where, if $q(t_k) \in \Omega_{\rho_{q,e}}$, then $q(t_{k+1}) \in \Omega_{\rho_q}$ for a nonlinear process-valve system under the controller of Equation (3.16). The role of the constraint of Equation (3.16f) is to allow for process economic optimization while maintaining the predicted process-valve state within $\Omega_{\rho_{q,e}}$, and the role of the constraint of Equation (3.16g) is to drive the process-valve state back into $\Omega_{\rho_{q,e}}$ when it exits this region. This combination of Equations (3.16f)–(3.16g) guarantees that the closed-loop state is maintained within Ω_{ρ_q} at all times if $q(t_0) \in \Omega_{\rho_q}$ and is driven to a neighborhood $\Omega_{\rho_{\min}}$ of the origin when $t > t_s$, as long as a feasible solution to the optimization problem exists at each sampling time and both Δ and θ are sufficiently small (in a sense that can be made precise in terms of a variety of functions and parameters related to the

LEMPC, system, and Lyapunov-based controller design (Heidarinejad *et al.*, 2012; Durand *et al.*, 2016); the fact that a sufficiently small θ is required for these theoretical results also motivates inclusion of valve dynamics in Equation (3.16b) to reduce plant-model mismatch). From the design of h_q to ensure that it satisfies Equation (3.16e), the design of Ω_{ρ_q} to ensure that the closed-loop state under $h_q(\tilde{q}(t_j))$, $t \in [t_j, t_{j+1})$, $j = k, \ldots, k+N-1$, satisfies Equation (3.16d), and the design of Equations (3.16f)–(3.16i) to be satisfied by $h_q(\tilde{q}(t_j))$, $t \in [t_j, t_{j+1})$, $j = k, \ldots, k+N-1$, h_q implemented in sample-and-hold is a feasible solution at every sampling time.

It is noted that Durand *et al.* (2016) and Durand and Christofides (2016) only consider $\epsilon_{r,1} = \epsilon_{r,2} = \cdots = \epsilon_{r,m} = \epsilon_r$ and $\epsilon_{desired,1} = \epsilon_{desired,2} = \cdots = \epsilon_{desired,m} = \epsilon_{desired}$. However, it is necessary to highlight the general case considered in this section where different upper bounds $\epsilon_{r,i}$ and $\epsilon_{desired,i}$ are allowed for each input $i = 1, \ldots, m$ (or to consider whether some other scaling of the components of u_m and of h_q in Equations (3.13) and (3.14) and Equations (3.16h) and (3.16i) can achieve a similar effect to allowing different upper bounds on each constraint while utilizing the same upper bounds). The reason for this is that the freedom to utilize different upper bounds for each input may aid in enhancing economic performance while still reducing wear. For example, for a single ϵ_r and $\epsilon_{desired}$ to sufficiently constrain all inputs (both those with large and small magnitudes) to prevent wear, ϵ_r and $\epsilon_{desired}$ may need to be small to prevent wear of valves with smaller flow rates out of them. This may limit the ability of the EMPC to enhance profits because it may cause those inputs with larger magnitudes to be able to change by relatively smaller percent deviations of $u_{m,i}$ from the prior values than if the magnitude of $u_{m,i}$ were smaller. However, Equations (3.16h) and (3.16i) are not required for proving closed-loop stability or robustness of the EMPC design of Equation (3.16) (Durand *et al.*, 2016; Durand and Christofides, 2016), but only for investigating feasibility. Since $h_q(\tilde{q}(t_j))$, $t \in [t_j, t_{j+1})$, $j = k, \ldots, k+N-1$, remains a feasible solution to Equations (3.16h) and (3.16i) for any upper bounds $\epsilon_{r,i} \geq 0$, $i = 1, \ldots, m$, having different upper bounds for each input poses no feasibility issues. Furthermore, through a direct extension of the results in Durand *et al.* (2016), it can be shown that Equations (3.13) and (3.14) are satisfied by the inputs computed by the controller of Equation (3.16) as long as Δ and $\epsilon_{r,i}$, $i = 1, \ldots, m$, are sufficiently small in the sense that:

$$2\epsilon_{r,i} + C_1\Delta \leq \epsilon_{desired,i}, \ \forall \ i = 1, \ldots, m, \tag{3.17}$$

where C_1 is a positive constant related to an upper bound on $|f(q, u_m, w)|$ and the maximum of all minimum Lipschitz constants that define the Lipschitz continuity of the $h_{q,i}$, $i = 1, \ldots, m$, in Ω_{ρ_q} (though it is possible to replace C_1 with a $C_{1,i}$, $i = 1, \ldots, m$, that depends on the minimum Lipschitz constant defining Lipschitz continuity for each $h_{q,i}$ rather than the maximum among all of those).

Note that even if the upper bounds on the input rate of change in Equations (3.16h) and (3.16i) are different for each input, Equation (3.17) requires that:

$$\Delta \leq \frac{\epsilon_{desired,i} - 2\epsilon_{r,i}}{C_1}, \ \forall \ i = 1, \ldots, m, \tag{3.18}$$

where Δ must be the same for all $i = 1, \ldots, m$. This means that despite the greater potential flexibility of the design with the upper bounds different for each i, Δ will still be fixed by the tightest difference between $\epsilon_{desired,i}$ and $2\epsilon_{r,i}$. It is the difference that fixes Δ, rather than the magnitude of each individually, so that Δ could potentially be fixed by an input for which a large $\epsilon_{desired,i}$ and $\epsilon_{r,i}$ are allowable if a tight tolerance is used between them (though if C_1 is replaced with $C_{1,i}$, then the tightest $\frac{\epsilon_{desired,i} - \epsilon_{r,i}}{C_{1,i}}$ fixes Δ). A motivation for using a tighter difference between $\epsilon_{desired,i}$ and $2\epsilon_{r,i}$ could be that a larger value of $\epsilon_{r,i}$ gives greater freedom to the LEMPC in choosing a control action to satisfy the constraints of Equations (3.16h) and (3.16i) and thus potentially to improve process profit; however, as indicated by this discussion, that benefit must be traded off with sampling period size. If it were desired to use different values of $\epsilon_{desired,i}$ (leading to different $\epsilon_{r,i}$) not only for different inputs but also across different sampling periods for the same input, care would have to be taken that any constraints enforced throughout the prediction horizon at a given sampling time are reflective of the actual constraints that will be enforced at those later sampling times to avoid plant-model mismatch.

Independent of the EMPC formulation utilized to attempt to enforce Equations (3.13) and (3.14) to account for valve wear is the underlying assumption that a relationship exists between $\epsilon_{desired,i}$, $i = 1, \ldots, m$, and the amount of wear experienced by a valve that can be used to tune the value of this parameter. However, because the input rate of change constraints do not explicitly model valve wear in a dynamic fashion, it may not be straightforward in general to choose appropriate values of $\epsilon_{r,i}$ and $\epsilon_{desired,i}$, $i = 1, \ldots, m$, to prevent wear. For example, EMPCs for two different processes may determine that cyclic input trajectories are optimal, but one may have a shorter period of the trajectory than the other so that one cyclic trajectory may wear valves more significantly than another due to frequency of input changes rather than magnitude. This suggests that it may not be effective to try to handle valve dynamics without explicitly modeling them at a fundamental enough level that constraint design becomes straightforward (e.g., for valve wear, modeling of the root issue causing wear, such as rubbing of materials, may be necessary to be able to develop appropriate constraints that are not difficult to tune; however, this remains an open research topic). Furthermore, Equations (3.13) and (3.14) constrain changes in u_m between sampling periods, which, when $u_a \neq u_m$, may not be as reflective of valve wear as constraining the maximum difference in u_a between two sampling periods with input rate of change constraints; restricting the rate of change of the actual valve output rather than its set-point, without impacting feasibility, could be investigated.

Example 2. Figure 3.2 demonstrates the use of input rate of change constraints in the EMPC of Equation (3.12) of the form of Equations (3.13) and (3.14) (with $N = N_k$) to control the process of Equations (3.7), (3.4)–(3.6), and (3.8)–(3.10) (the trajectories for u_a, u_m, and P in this case are denoted by "EMPC-C"). The upper bound $\epsilon_{desired}$ is taken to be 0.1 throughout the prediction horizon (the constraints of Equations (3.13) and (3.14) were implemented rather than constraints designed to guarantee feasibility in LEMPC; because no Lyapunov-based stability constraints are used in Figure 3.2, these results are not LEMPC-specific). It can be seen from Figure 3.2a that the input rate of change constraints prevent u_m from changing by more than 0.1 between two sampling periods (which prevents drastic changes in u_a as well and therefore may help to prevent valve wear), and for this example, that had an impact on preventing the pressure from the pneumatic actuation from becoming saturated as often as if the valve output flow rate set-points were less constrained. This example demonstrates that feasibility issues can occur if constraints are not accounted for in the EMPC design stage carefully, because EMPC-C was infeasible for three of the sampling periods depicted in the figure.

3.1.2 EMPC accounting for valve behavior: Impacts of valve behavior on ease of design

In this section, we consider how accounting for valve behavior in EMPC can impact the readiness with which an EMPC formulation in the literature can be designed for process-valve systems. To investigate this, we analyze three recent LEMPC formulations (for consistency with the description of LEMPC for process-valve systems in the prior sections) which were developed to handle practical issues (meeting a production schedule and reducing the computation time of EMPC) for nonlinear chemical process systems. Through these formulations, we demonstrate that implementation difficulties may arise when accounting for valve dynamics in EMPC formulations in the literature due to the form of models for valve behavior. The goal is not to provide an exhaustive review of the challenges with adjusting all EMPC formulations to account for process-valve dynamics, but rather to use several illustrative examples to highlight the need for future EMPC designs to consider valve behavior from the beginning of design.

Impacts of Valve Behavior on Ease of EMPC Design: Steady-State Determination. The first formulation to be described is an LEMPC tailored to handle production management considerations (Alanqar *et al.*, 2017a). Specifically, the LEMPC is designed to drive certain components of the system state to values determined by a production scheduling algorithm. Though this formulation did not consider valve dynamics or input rate of change constraints in Alanqar *et al.* (2017a), we present here an extension that accounts for a process-valve model and input rate of change constraints (the input rate of change constraints are used here as the best available method in the EMPC literature for accounting for the dynamics of valve wear, despite their limitations as described in the prior section). In this case, we denote the components of the state vector that are required to reach specific values ("scheduled" states) by q_i, $i = 1, \ldots, n_s$, $n_s \leq n$. The LEMPC for production management is therefore developed as follows:

$$\min_{u_m(t) \in S(\Delta)} \int_{t_k}^{t_{k+N}} [L_e(\tilde{q}(\tau), u_m(\tau)) + \sum_{i=1}^{n_s} \alpha_{Wi}(\tilde{q}_i(\tau))^2] d\tau \tag{3.19a}$$

$$\text{s.t.} \quad \dot{\tilde{q}}(t) = f(\tilde{q}(t), u_m(t)) \tag{3.19b}$$

$$\tilde{q}(t_k) = q(t_k) \tag{3.19c}$$

$$\tilde{q}(t) \in Q, \forall\, t \in [t_k, t_{k+N}) \tag{3.19d}$$

$$u_m(t) \in U_m, \ \forall\, t \in [t_k, t_{k+N}) \tag{3.19e}$$

$$V_q(\tilde{q}(t)) \leq \rho_{q,e}, \ \forall \ t \in [t_k, t_{k+N}), \ \text{if } V_q(q(t_k)) \leq \rho_{q,e} \tag{3.19f}$$

$$\frac{\partial V_q(q(t_k))}{\partial q} f(q(t_k), u_m(t_k)) \leq \frac{\partial V_q(q(t_k))}{\partial q} f(q(t_k), h_q(q(t_k))),$$
$$\text{if } t_k > t_s \text{ or } V_q(q(t_k)) > \rho_{q,e} \text{ or } |q_i(t_k)| \geq \gamma_i,$$
$$i = 1, \ldots, n_s \tag{3.19g}$$

$$|u_{m,i}(t_k) - h_{q,i}(q(t_k))| \leq \epsilon_{r,i}, \ \forall \ i = 1, \ldots, m \tag{3.19h}$$

$$|u_{m,i}(t_j) - h_{q,i}(\tilde{q}(t_j))| \leq \epsilon_{r,i}, \ \forall \ i = 1, \ldots, m,$$
$$j = k+1, \ldots, k+N-1, \tag{3.19i}$$

where α_{Wi} is the penalty on the deviation of the i-th state, $i = 1, \ldots, n_s$, of the process-valve model from its steady-state value, and the γ_i, $i = 1, \ldots, n_s$, represent upper bounds on the absolute values of the deviations of the measured values of the n_s scheduled states from their steady-state values. The roles of the constraints are similar to those in Equation (3.16), with the modification that Equation (3.19g) is activated under an additional condition that $|q_i(t_k)| \geq \gamma_i, \ i = 1, \ldots, n_s$, so that the value of the Lyapunov function along the closed-loop state trajectories decreases between two sampling periods when any q_i, $i = 1, \ldots, n_s$, is not within γ_i of its scheduled value. This is done because it is assumed that each

q_i, $i = 1, \ldots, n_s$, can be driven within γ_i of its scheduled value under repeated application of Equation (3.19g). The steady-state can be made to vary over time in accordance with the production schedule, and Alanqar *et al.* (2017a) discuss methods for guaranteeing that the closed-loop state is driven from one steady-state to the next without losing closed-loop stability or feasibility of the optimization problem.

The primary difference between Equation (3.19) and the LEMPC for production management formulation in Alanqar *et al.* (2017a) is the input rate of change constraints in Equations (3.19h) and (3.19i). It can be readily verified, however, that because Equation (3.16) and (3.19) have identical constraints (i.e., the only difference is in the activation condition for Equation (3.16g) but not in its form), the closed-loop stability, feasibility, and input rate of change results described in the prior section for Equation (3.16) hold for Equation (3.19) as well (as long as all sufficient conditions and assumptions required for the theoretical results hold). Therefore, though this analysis indicates that some additional investigation is required to evaluate the properties of an EMPC formulation in the literature that is being extended to account for valve behavior through constraints such as input rate of change constraints, in many cases, it may be possible to accomplish such an analysis fairly quickly through analogy of new LEMPC formulations with those for which valve behavior was explicitly considered.

However, this concept that an EMPC which does not account for valve behavior can be extended, in a straightforward fashion, to account for such behavior ignores the fact that there can be fundamental differences in the dynamics of equipment compared to the dynamics of chemical processes that may affect whether critical assumptions utilized in designing an EMPC for a nonlinear process system can be verified to hold if that design is utilized for a process-equipment system. An example of fundamental differences between equipment behavior and process behavior is valve saturation. It would be rare to find a chemical process with such a non-differentiable nonlinearity; however, because equipment is physically limited, saturation nonlinearities are common when valve dynamics are considered. Assumptions 1–2 are important in Equation (3.16) and are critical to the entire concept behind Equation (3.19), requiring that a steady-state for the system can be located and characterized, and that the closed-loop state can be driven to this steady-state and, in the case of Equation (3.19), can be driven from a region around one steady-state to a region around a different steady-state if required by the schedule. For chemical processes, such assumptions are generally considered to be non-limiting (i.e., they hold for most chemical process systems of interest). However, it may be more difficult to verify these assumptions when valve behavior is included.

To demonstrate this, consider the process-valve system from Durand *et al.* (2017) defined by Equations (3.4)–(3.6) and the following equation which describes the dynamics of the level h_E in a tank:

$$\frac{dh_E}{dt} = \frac{1}{A_E}\left(\left(\frac{x_{v,\max} - x_v}{x_{v,\max}}\right)u_{a,\max} - c_1\sqrt{h_E}\right), \tag{3.20}$$

where A_E is the tank cross-sectional area and c_1 is the resistance coefficient. The level can be controlled by manipulating the pressure applied to a sticky pneumatic sliding-stem globe valve that opens and closes to allow more or less flow, respectively, into the tank. If it is considered desirable to develop an LEMPC to determine the pressure, then a steady-state must be determined. If the right-hand side of each differential equation of the model is set to zero, the result indicates that a value of x_v can be determined for a desired value of h_E, $v_v = 0$, and $A_vP = \sigma_0 z_f + k_s x_v$. However, this last equality implies that to drive the level to a certain value, any value of z_f that is related to the input P through this equality can be associated with the desired value of the level. Even if an explicit controller were utilized to control the process, as required in developing h_q for the LEMPC, the steady-state value of z_f can remain unclear because at steady-state, $v_v = 0$, which always causes Equation (3.6) to provide no information on the value of z_f, and additional analysis would be required to determine if a steady-state exists or not.

One method for analyzing this issue further would be to replace the friction model with one which does not contain any states for the friction model like z_f for which an engineer would not have an exact steady-state value in mind. For example, the classical model (Garcia, 2008) could be utilized instead, resulting in the dynamic system of Equations (3.4), (3.6), and (3.20) combined with the following expression for the valve velocity:

$$\frac{dv_v}{dt} = \begin{cases} \frac{1}{m_v}[A_vP - k_sx_v - (F_C + (F_S - F_C)e^{-(v_v/v_s)^2})sgn(v_v) - \sigma_2 v_v], \\ \qquad\qquad\qquad\qquad\qquad \text{if } v_v \neq 0 \\ 0 \qquad\qquad\qquad\qquad\qquad \text{if } v_v = 0 \text{ and } |A_vP - k_sx_v| \leq F_S \\ \frac{1}{m_v}[A_vP - k_sx_v - F_S sgn(A_vP - k_sx_v)], \\ \qquad\qquad\qquad\qquad\qquad \text{if } v_v = 0 \text{ and } |A_vP - k_sx_v| > F_S \end{cases} \tag{3.21}$$

Again, the issue of isolation comes up for the open-loop process-valve system because the steady-state values of x_v, h_E, and v_v occur for a number of different P values (i.e., any for which $|A_vP - k_sx_v| \leq F_S$). The equation $\frac{dv_v}{dt} = 0$ in Equation (3.21) associated with the loss of isolation of a steady-state does not allow the right-hand side to be determined as a function of P, and therefore there is no control law that can alter the dynamics of v_v until $|A_vP - k_sx_v| > F_S$ unless it is able to cause them to be bypassed by causing $|A_vP - k_sx_v|$ to never be less than or equal to F_S whenever a new set-point for the level is requested.

The above analysis indicates that the nonlinearities which describe certain types of valve dynamics may make it more difficult to find appropriate stabilizing controllers or steady-states for process-valve systems than for a standard chemical process. This indicates that neglecting valve dynamics at the design stage of an EMPC formulation may cause important directions to be missing from the literature regarding how to appropriate such designs to cases where valve-related nonlinearities make the design of the controller's constraints challenging. Even more fundamentally, it must be analyzed whether it is possible to develop EMPC formulations with isolated steady-states to which the closed-loop state can be driven over time (this is important to a number of EMPC formulations and is not limited to LEMPC) with control-relevant process-valve models, and if not, what types of constraints or theory can be utilized to handle process-valve systems. Furthermore, differentiability of the objective function and constraints of an EMPC when process-valve models are utilized should be investigated to aid in appropriate choices of optimization algorithms. There may also be techniques for handling some valve nonlinearities outside the process model in EMPC. For example, if saturation of a state is a concern, then rather than modeling the saturation of the state in the process-valve model, a state constraint can be added to the optimization problem (Durand *et al.*, 2017).

Impacts of Valve Behavior on Ease of EMPC Design: Empirical Modeling and Distributed Control. The two example designs which will be analyzed in this section have particular relevance for EMPC incorporating process-valve dynamics because they focus on computation time reduction (Fang and Armaou, 2016), and incorporating valve dynamics within the process model increases the number of states of the dynamic model, which would be expected to increase computation time. Further motivation for attempting to reduce computation time is that reducing the sampling time for a process-valve system may allow the controller to be more flexible to handle the nonlinearities of stiction. For example, in Durand *et al.* (2017), it is noted that the sampling period of an EMPC that includes the process-valve dynamics for a valve without flow control is significantly longer than the time-scale on the which valve slips, with the result that the controller cannot adjust the valve position while the valve is slipping, which can prevent it from being able to smoothly drive the process state to its set-point. Utilizing a very short sampling period was postulated to be a method for improving these results.

The first example design considered is that for LEMPC with an empirical model used for making state predictions instead of a first-principles model (Alanqar *et al.*, 2015a; Alanqar *et al.*, 2015b). This formulation has been developed for input-affine nonlinear systems with the following form (written here for a process-valve system):

$$\dot{q}(t) = f_p(q(t), w(t)) + \tilde{G}(q(t), w(t))u_m(t), \tag{3.22}$$

where f_p and $\tilde{G}$ are nonlinear vector and matrix functions, respectively, which are infinitely differentiable and can be locally expressed with a convergent power series. Equation (3.22) is a member of the class of systems of Equation (2.1).

It is assumed that either the nonlinear model of Equation 3.22 is unavailable or that it is desirable not to use the nonlinear model in EMPC for computation time reasons, but to instead use an empirical model with the following form:

$$\dot{\hat{q}}(t) = A\hat{q}(t) + P_z(\hat{q}(t)) + Bu_m(t), \tag{3.23}$$

where A and B are matrices of constant coefficients, $\hat{q}$ denotes the state of the process-valve system as determined from the empirical model, and $P_z(\hat{q})$ is a vector function containing nonlinear monomial terms in the components of $\hat{q}$ of order two to order z, i.e., $P_z(\hat{q}) := E\zeta_{NL}(\hat{q})$, $\zeta_{NL}(\hat{q}) = [\hat{q}_1^2 \; \hat{q}_1\hat{q}_2 \; \cdots \; \hat{q}_n^z]^T$, with E denoting a matrix of coefficients of the terms in $\zeta_{NL}(\hat{q})$. The following LEMPC formulation is developed with an empirical model utilized for making state predictions:

$$\min_{u_m(t)\in S(\Delta)} \int_{t_k}^{t_{k+N}} L_e(\tilde{\hat{q}}(\tau), u_m(\tau))\, d\tau \tag{3.24a}$$

$$\text{s.t.} \quad \dot{\tilde{\hat{q}}}(t) = A\tilde{\hat{q}}(t) + P_z(\tilde{\hat{q}}(t)) + Bu_m(t) \tag{3.24b}$$

$$\tilde{\hat{q}}(t_k) = q(t_k) \tag{3.24c}$$

$$\tilde{\hat{q}}(t) \in Q, \forall\, t \in [t_k, t_{k+N}) \tag{3.24d}$$

$$u_m(t) \in U_m, \;\; \forall\, t \in [t_k, t_{k+N}) \tag{3.24e}$$

$$\hat{V}_q(\tilde{\hat{q}}(t)) \le \rho_{\hat{q},e}, \;\; \forall\; t \in [t_k, t_{k+N}), \;\; \text{if } \hat{V}_q(q(t_k)) \le \rho_{\hat{q},e} \tag{3.24f}$$

$$\frac{\partial \hat{V}_q(q(t_k))}{\partial q}(Bu_m(t_k)) \le \frac{\partial \hat{V}_q(q(t_k))}{\partial q}(Bh_{\hat{q}}(q(t_k))), \quad \text{if } t_k > t_s \text{ or } \hat{V}_q(q(t_k)) > \rho_{\hat{q},e}, \tag{3.24g}$$

where the notation follows along the lines of that in Equation (3.16), with $\tilde{\hat{q}}$ representing the prediction of the process state obtained from the empirical model, and $\hat{V}$ and $h_{\hat{q}}$ representing the Lyapunov function and Lyapunov-based controller obtained based on the empirical model (i.e., $\hat{V}$ satisfies constraints similar to, but stronger than, those in Assumption 2 when $h_{\hat{q}}$ is used to control the process of Equation 3.23; a number of additional conditions are also required for the stability and feasibility results in Alanqar *et al.*, 2015a; Alanqar *et al.*, 2015b). $\rho_{\hat{q}_e}$ is an upper bound on the Lyapunov function value that, like ρ_e in Equation (3.16), is used to determine which of the Lyapunov-based stability constraints in Equation (3.24) is enforced at a given sampling time.

One of the fundamental assumptions underlying both the practical use of Equation (3.24) and also the theory related to this formulation in Alanqar *et al.* (2015a) and Alanqar *et al.* (2015b) is that modeling the dynamics of a system using the form of Equation (3.23) is reasonable. As shown in the prior section, process-valve models may contain nonlinearities due to the valve dynamics with a different character than those typically observed for chemical processes. For example, it has been suggested in a number of works (e.g., Durand *et al.*, 2017; Choudhury *et al.*, 2005; He *et al.*, 2007; Kano *et al.*, 2004) that an empirical model for stiction be formed with an "if-then" type structure (i.e., the manner in which the valve output changes in response to changes in the control signal received by the valve may be different based on conditions such as the magnitude of the change in the control signal). This implies that a single differential equation with polynomial terms may not be sufficient for representing all valve behavior. Since the process and valve behavior are coupled, this could also prevent the process-valve model from taking the form of Equation (3.23), and should therefore be investigated. This discussion exemplifies the need to consider valve behavior from the beginning of EMPC design to verify whether the fundamental assumptions of the EMPC methods developed and their theoretical results (which depend on factors such as the assumed form of the class of systems) will be applicable to the physical process-equipment systems to which they will be applied, and to address explicitly how to handle cases where they are not or where it is not clear if they are.

The second computation time reduction method to be described in this section is a distributed LEMPC (DLEMPC) formulation (i.e., the m process inputs are computed by $\bar{m}$ distributed controllers instead of by a single centralized controller, where the i-th distributed controller solves for a subset of the available process inputs denoted by $\bar{u}_{m,i}$, $i = 1, \ldots, \bar{m}$). Two types of DLEMPC designs (termed "sequential" and "iterative" designs) have been developed for input-affine nonlinear systems with the following form (here written for a process-valve system):

$$\dot{q}(t) = \tilde{f}(q(t)) + \sum_{i=1}^{\bar{m}} g_i(q(t))\bar{u}_{m,i}(t) + b(q(t))w(t), \tag{3.25}$$

where the vector functions $\tilde{f}$, g_i, $i = 1, \ldots, \bar{m}$, and b are locally Lipschitz and $\bar{u}_i$ denotes one of $\bar{m}$ vectors containing m_i process inputs from the input vector u_m, where $m = \sum_{i=1}^{\bar{m}} m_i$.

In a sequential DLEMPC, $\bar{m}$ controllers solve for subsets of the total number (m) of control inputs available (specifically, each solves for m_i inputs, $i = 1, \ldots, m_{\bar{m}}$) in sequence. The i-th DLEMPC in the sequence receives the input trajectories computed by the $i-1$ DLEMPCs before it in the sequence (i.e., it receives trajectories for $\sum_{j=1}^{i-1} m_j$ inputs) and assumes that the $m_{i+1}, \ldots, m_{\bar{m}}$ inputs are equal to the corresponding components of h_q implemented in sample-and-hold. The following is the formulation of a sequential DLEMPC (Chen *et al.*, 2012; Albalawi *et al.*, 2017a):

$$\min_{\bar{u}_m(t)\in S(\Delta)} \int_{t_k}^{t_{k+N}} L_e(\tilde{q}^j(\tau), \bar{u}_{m,1}(\tau), \ldots, \bar{u}_{m,\bar{m}}(\tau))\, d\tau \tag{3.26a}$$

$$\text{s.t.} \quad \dot{\tilde{q}}^j(t) = \tilde{f}(\tilde{q}^j(t)) + \sum_{i=1}^{\bar{m}} g_i(\tilde{q}^j(t))\bar{u}_{m,i}(t) \tag{3.26b}$$

$$\tilde{q}^j(t_k) = q(t_k) \tag{3.26c}$$

$$\tilde{q}^j(t) \in Q, \, \forall\, t \in [t_k, t_{k+N}) \tag{3.26d}$$

$$\bar{u}_{m,j}(t) \in \bar{U}_{m,j}, \;\; \forall\, t \in [t_k, t_{k+N}) \tag{3.26e}$$

$$\bar{u}_{m,r}(t) = \bar{h}_{q,r}(\tilde{q}^j(t_p)), \;\; r = j+1, \ldots, \bar{m}, \;\; \forall\, t \in [t_p, t_{p+1}), \quad p = k, \ldots, k+N-1 \tag{3.26f}$$

$$\bar{u}_{m,s}(t) = \bar{u}^*_{m,s}(t|t_k), \;\; s = 1, \ldots, j-1, \;\; \forall\, t \in [t_k, t_{k+N}) \tag{3.26g}$$

$$V_q(\tilde{q}^j(t)) \leq \rho_{q,e}, \;\; \forall\; t \in [t_k, t_{k+N}), \;\; \text{if } V(q(t_k)) \leq \rho_{q,e} \tag{3.26h}$$

$$\frac{\partial V_q(q(t_k))}{\partial q}\left(\sum_{i=1}^{\bar{m}} g_i(\tilde{q}^j(t))\bar{u}_{m,i}(t)\right)$$
$$\leq \frac{\partial V_q(q(t_k))}{\partial q}\left(\sum_{i=1}^{\bar{m}} g_i(\tilde{q}^j(t))\bar{h}_{q,i}(q(t_k))\right),$$
$$\text{if } t_k > t_s \text{ or } V_q(q(t_k)) > \rho_{q,e} \tag{3.26i}$$

where the notation follows that in Equation (3.16) and $\tilde{q}^j$ is the predicted state trajectory according to Equation (3.26b) within the j-th DLEMPC. $\bar{U}_{m,j}$ represents the input constraints on $\bar{u}_{m,j}$ (obtained from the appropriate constraints in U and considering $u_{a,i}^{\min} = -u_{a,i}^{\max}$) and $\bar{h}_{q,i}(q(t_k))$ represents the vector of components of $h_q(q(t_k))$ corresponding to the m_i inputs in $\bar{u}_i$.

In contrast to a sequential DLEMPC, in an iterative DLEMPC architecture, the $\bar{m}$ controllers are solved simultaneously for their respective subsets of the m components of the input vector (determining the solutions of all distributed controllers is referred to as an iteration). At the first iteration, each DLEMPC assumes that the inputs for which it does not solve are fixed to the appropriate components of h_q implemented in sample-and-hold. Once solutions to all DLEMPCs have been obtained, the DLEMPCs can communicate their solutions to one another and perform additional iterations. During subsequent iterations, the i-th DLEMPC, $i = 1, \ldots, \bar{m}$, solves only for m_i inputs and assumes that the remaining inputs are fixed to the solutions determined by the other DLEMPC's at the prior iteration. The formulation of the j-th iterative DLEMPC is that of Equation (3.26) but with the following equations used in place of Equations (3.26f) and (3.26g) (Liu *et al.*, 2010; Albalawi *et al.*, 2017a):

$$\bar{u}_{m,r}(t) = \bar{h}_{q,r}(\tilde{q}^j(t_p)),\ r \in \{1, \ldots, \bar{m}\}, r \neq j,\ \forall\, t \in [t_p, t_{p+1}),$$
$$p = k, \ldots, k+N-1,\ c = 1 \tag{3.27a}$$
$$\bar{u}_{m,r}(t) = \bar{u}^*_{m,r,c-1}(t|t_k),\ r \in \{1, \ldots, \bar{m}\},\ r \neq j,\ \forall\, t \in [t_p, t_{p+1}),$$
$$p = k, \ldots, k+N-1,\ c \geq 2 \tag{3.27b}$$

and the following equation used in place of Equation (3.26i):

$$\frac{\partial V_q(q(t_k))}{\partial q} g_j(q(t_k))\bar{u}_j(t_k) \leq \frac{\partial V_q(q(t_k))}{\partial q} g_j(q(t_k))\bar{h}_{q,j}(q(t_k)),$$
$$\text{if } t_k > t_s \text{ or } V_q(q(t_k)) > \rho_{q,e} \qquad (3.28)$$

In Equations (3.27a) and (3.27b), c signifies the iteration number, and $\bar{u}^*_{m,r,c-1}(t|t_k)$, $t \in [t_k, t_{k+N})$, signifies the optimal solution from the r-th DLEMPC at iteration $c-1$.

The two DLEMPC designs provide an effective framework for demonstrating that despite the relative ease with which both the formulation of an LEMPC accounting for valve behavior and the theoretical results for such an LEMPC were obtained for Equation (3.19) by directly extending the results in Durand *et al.* (2016) and Durand and Christofides (2016) to account for valve behavior (in that case, through input rate of change constraints), extending other EMPC results in the literature to account for valve behavior, even through the same constraints, can require more careful analysis and new constraint designs, making the results without accounting for valve behavior in such cases incomplete and therefore reducing their utility. To demonstrate this, we first consider the design and theoretical developments required to extend sequential and iterative DLEMPCs to handle input rate of change constraints. This discussion relies on the results obtained in (Liu *et al.*, 2010; Albalawi *et al.*, 2017a; Chen *et al.*, 2012) for distributed LEMPC without input rate of change constraints. The important results from those works for the sequential design for this discussion are summarized as follows: 1) $\bar{h}_{q,j}(\tilde{q}^j(t_p))$, $t \in [t_p, t_{p+1})$, $p = k, \ldots, k+N-1$, is a feasible solution to the j-th sequential DLEMPC because it satisfies all state and input constraints in Equation (3.26); 2) when the DLEMPC of Equation (3.26) is feasible, the inputs computed by the $\bar{m}$ sequential DLEMPC's maintain the closed-loop state of Equation (3.25) within Ω_{ρ_q} at all times (under sufficient conditions and assumptions). If it is desired to add input rate of change constraints, however, consideration must be given to the fact that Equations (3.16h) and (3.16i) apply to all manipulated inputs, but only a subset of the manipulated inputs is available to be computed in each sequential DLEMPC. Therefore, the following input rate of change constraints must be added to the j-th

DLEMPC for all i between 1 and m that correspond to the inputs in $\bar{u}_{m,j}$ (i.e., there should be m_j sets of constraints of the following form):

$$|u_{m,i}(t_k) - h_{q,i}(q(t_k))| \leq \epsilon_{r,i} \tag{3.29a}$$

$$|u_{m,i}(t_p) - h_{q,i}(\tilde{q}^j(t_p))| \leq \epsilon_{r,i},\ p = k+1, \ldots, k+N-1 \tag{3.29b}$$

The two feasibility/stability points described from Liu *et al.* (2010), Albalawi *et al.* (2017a), and Chen *et al.* (2012) continue to hold when these input rates of change constraints are applied because $\bar{h}_{q,j}(\tilde{q}^j(t_p))$, $t \in [t_p, t_{p+1})$, $p = k, \ldots, k+N-1$, remains a feasible solution to these constraints. Similarly, Equations (3.13) and (3.14) will hold for all m inputs applied to the process if Equation (3.17) holds since Equations (3.29a) and (3.29b) are feasible.

The constraints of Equations (3.29a) and (3.29b) are also appropriate for the j-th DLEMPC, for all $i \in \{1, \ldots, m\}$ that correspond to the inputs in the vector $\bar{u}_{m,j}$ (rather than Equations (3.16h) and (3.16i)). The relevant feasibility and stability properties for this discussion from Albalawi *et al.* (2017a), which hold under appropriate assumptions and conditions, are: 1) $\bar{h}_{q,j}(\tilde{q}^j(t_p))$, $t \in [t_p, t_{p+1})$, $p = k, \ldots, k+N-1$, is a feasible solution to each iterative DLEMPC for $c = 1$; 2) for a feasible solution to each iterative DLEMPC to exist if $c > 1$, it must be checked that V_q remains below $\rho_{q,e}$ when V_q is computed along the closed-loop state trajectory of Equation (3.25) with $w \equiv 0$ and inputs $\bar{u}^*_{m,r,c-1}(t|t_k)$, $t \in [t_k, t_{k+N})$, $r = 1, \ldots, \bar{m}$. The resulting feasible solution at iteration c in the j-th DLEMPC (if this condition on V_q is met) is then $\bar{u}^*_{m,j,c-1}(t|t_k)$, $t \in [t_k, t_{k+N})$; and 3) the closed-loop state is maintained within Ω_{ρ_q} if, at each sampling time, either a feasible solution to all $\bar{m}$ DLEMPCs that also meets the requirement on V_q is applied to the process or $h_q(q(t_k))$ is applied if the solution returned at $c = 1$ does not meet the requirement on V_q at $c = 1$. The analysis of whether these three conditions continue to hold, and also Equations (3.13) and (3.14), when Equations (3.29a) and (3.29b) are included in the j-th DLEMPC requires analyzing feasibility of each iteration with these constraints and also the closed-loop state and input trajectories under the potential combination of $h_q(q(t_k))$ and the feasible DLEMPC solutions that meet the V_q requirement that may be applied to the process over time. Specifically, when $c = 1$, $\bar{h}_{q,j}(\tilde{q}^j(t_p))$, $t \in [t_p, t_{p+1})$, $p = k, \ldots, k+N-1$, remains a feasible solution to the constraints in each DLEMPC since it satisfies Equations (3.29a) and (3.29b). If a subsequent iteration is performed, $\bar{u}^*_{m,j,c-1}(t|t_k)$, $t \in [t_k, t_{k+N})$ is a feasible solution if the V_q requirement was met because it satisfied Equations (3.29a) and (3.29b) at iteration $c-1$ and therefore will satisfy them at iteration c as well.

Finally, though the added Equations (3.29a) and (3.29b) will not affect the stability proof, it must be analyzed whether they guarantee that Equations (3.13) and (3.14) are met when Equation (3.17) holds, at every sampling time, regardless of whether the DLEMPC inputs or $h_q(q(t_k))$ is applied to the process (in particular, whether Equation (3.13) on the applied inputs is always satisfied, and whether at a given sampling time where the DLEMPC solution is applied, whether Eq. 3.14 holds on all non-implemented inputs computed by the DLEMPC). Upper bounds on Equations (3.13) and (3.14) for each $i = 1, \ldots, m$ and $j = k+1, \ldots, k+N-1$ are, respectively (Durand *et al.*, 2014):

$$|u^*_{m,i}(t_k|t_k) - h_{q,i}(q(t_k))| + |u^*_{m,i}(t_{k-1}|t_{k-1}) - h_{q,i}(q(t_{k-1}))| \\ + |h_{q,i}(q(t_k)) - h_{q,i}(q(t_{k-1}))| \tag{3.30a}$$

$$|u^*_{m,i}(t_j|t_k) - h_{q,i}(\tilde{q}^j(t_j))| + |u^*_{m,i}(t_{j-1}|t_k) - h_{q,i}(\tilde{q}^j(t_{j-1}))| \\ + |h_{q,i}(\tilde{q}^j(t_j)) - h_{q,i}(\tilde{q}^j(t_{j-1}))| \tag{3.30b}$$

Conditions which allow Equations (3.13) and (3.14) to hold if Equation (3.17) forms an upper bound on these equations are: Condition 1) $|u^*_{m,i}(t_j|t_k) - h_{q,i}(\tilde{q}^j(t_j))| \le \epsilon_{r,i}$, $i = 1, \ldots, m$, $j = k, \ldots, k+N-1$; Condition 2) $|u^*_{m,i}(t_{k-1}|t_{k-1}) - h_{q,i}(q(t_{k-1}))| \le \epsilon_{r,i}$, $i = 1, \ldots, m$ (to ensure there is no ambiguity at t_0, set $u^*_{m,i}(t_0|t_0) = h_{q,i}(q(t_0))$, $i = 1, \ldots, m$). If the LEMPC solution is applied to the process-valve system, Equations (3.29a) and (3.29b) are feasible and therefore Condition 1 holds. Condition 1 is trivially satisfied using $h_{q,i}(q(t_k))$, $i = 1, \ldots, m$, as the system input for $t_j = t_k$. Finally, whether $u^*_{m,i}(t_{k-1}|t_{k-1})$ came from a feasible solution to the DLEMPC optimization problem or from $h_{q,i}(q(t_{k-1}))$, Condition 2 is satisfied. Therefore, Equation (3.13) is satisfied by the input trajectory applied to the process under the iterative DLEMPC implementation strategy over time. This discussion regarding how to extend the iterative and sequential designs indicates that updating EMPC designs to account for valve behavior may require new constraints to be developed for a design and new theoretical analysis if the valve behavior is not accounted for from the beginning of the design.

3.2 EMPC accounting for equipment behavior

Motivated by the importance of including valve behavior in EMPC as reviewed in the prior sections, we conclude by proposing that other equipment dynamics, also traditionally neglected when modeling processes and designing controllers, may be critical to account for within EMPC design, again from the design stage. Equipment-related considerations (e.g., corrosion Finšgar and Jackson, 2014; Garcia-Arriaga *et al.*, 2010; Anderko *et al.*, 2005), heat exchanger fouling (Yeap *et al.*, 2004; Bohnet, 1987; Polley *et al.*, 2002), catalyst fouling (Pacheco and Petersen, 1984; Zhang and Seaton, 1996), fatigue (Okrajni *et al.*, 2005), creep (Ul-Hamid *et al.*, 2006; Bonaccorsi *et al.*, 2014), impeller wear (Aiming *et al.*, 1995), pump leakage (Khan and Abbasi, 2001), and sensor drift (Center for Chemical Process Safety, 2017), all of which are observed in the chemical process industries) can be impacted by and/or may themselves impact process operating conditions. Therefore, one could consider that an MPC/EMPC should be made aware of the dynamics of equipment through a process-equipment model. This can be expected to be beneficial for two major reasons: 1) EMPC may operate processes in ways that they have not been operated before (i.e., with persistent time-varying operation as opposed to steady-state operation). It is not then obvious whether or not new equipment concerns may arise (e.g., shorter time to failure of equipment (Kidam and Hurme, 2013) due to the manner in which the equipment is impacted by the operating strategy over time) if the EMPC is not aware of the equipment behavior. This is especially important to address because it is not possible to predict the manner in which an EMPC may operate a process *a priori*, especially in the presence of disturbances. 2) The purpose of utilizing EMPC to control a process is to enhance profit, and equipment replacement due to changes in the equipment over time can decrease profit. It is necessary to investigate whether an EMPC can enhance process profits during operation while simultaneously decreasing equipment costs by being made aware of equipment limitations (this may be beneficial for tracking MPC as well).

The first step in enabling this vision of an EMPC which accounts for equipment behavior is selecting and/or developing sufficiently accurate, control-relevant models for equipment behavior which can effectively represent any coupling between the dynamics of a process and of equipment. These models must be capable of predicting equipment dynamics regardless of the operating conditions or changes in operating conditions (e.g., a model for creep developed from data at a fixed temperature may not be sufficient). This will require an analysis of literature on a variety of different dynamic equipment considerations. It will also require models to be selected that can accurately account for multiple types of equipment behavior occurring at once (e.g., corrosion in addition to creep). Finally, it will require methods for determining how to incorporate the models in EMPC in a manner that allows all potential equipment dynamics to be accounted for, even those which may not be thought of as applying to a given process, due to the inability to predict *a priori* how an EMPC may control a process and thus an inability to pre-determine all possible equipment dynamics that may have significance within the process–equipment model.

However, determining an appropriate process–equipment model is just the first step in working to achieve EMPC designs that explicitly account for the interactions between processes and equipment. As for the case when sticky valves are the types of equipment under focus, new constraints may be required (e.g., constraints on the rate of corrosion or the stress experienced by a component), which will need to be developed and incorporated within EMPC from the beginning of design. Accounting for equipment dynamics from the beginning of EMPC design may also expose, as for the valves, a need to question whether fundamental assumptions of traditional EMPC design techniques which neglected equipment dynamics continue to hold when process–equipment systems are considered. For example, advances in EMPC focused on operational safety (Kletz, 2009; Khan and Abbasi, 1999; Pariyani *et al.*, 2010) have introduced the concept that safety is related to the process state and may be quantified through a state-based metric termed the Safeness Index $S(\cdot)$ upon which a threshold value can be set to delineate between states which are acceptable to operate at and those which are not desirable from a safety perspective (Albalawi *et al.*, 2017b). An LEMPC formulation was developed that can drive the state from any $q(t_k) \in \Omega_{\rho_q}$ into the region where $S(\cdot)$ is less than its threshold in finite time (under sufficient conditions and assumptions) as follows (extended here to process–valve systems):

$$\max_{u_m(t)\in S(\Delta)} \int_{t_k}^{t_{k+N}} L_e(\tilde{q}(\tau), u_m(\tau))\, d\tau \tag{3.31a}$$

$$\text{s.t. } \dot{\tilde{q}}(t) = f(\tilde{q}(t), u_m(t)) \tag{3.31b}$$

$$\tilde{q}(t_k) = q(t_k) \tag{3.31c}$$

$$\tilde{q}(t) \in Q,\ \forall\, t \in [t_k, t_{k+N}) \tag{3.31d}$$

$$u_m(t) \in U_m,\ \forall\, t \in [t_k, t_{k+N}) \tag{3.31e}$$

$$V_q(\tilde{q}(t)) \le \rho_{q,e},\ \forall\, t \in [t_k, t_{k+N}) \quad \text{if } V_q(q(t_k)) \le \rho_{q,e} \tag{3.31f}$$

$$S(\tilde{q}(t)) \le S_{TH},\ \forall\, t \in [t_k, t_{k+N}) \quad \text{if } S(q(t_k)) \le S_{TH} \tag{3.31g}$$

$$\frac{\partial V_q(q(t_k))}{\partial q} f(q(t_k), u_m(t_k)) \le \frac{\partial V_q(q(t_k))}{\partial q} f(q(t_k), h_q(q(t_k))), \quad \text{if } V_q(q(t_k)) > \rho_{q,e} \text{ or } t_k > t_s \text{ or } S(q(t_k)) > S_{TH} \tag{3.31h}$$

where the notation follows that in Equations (2.2) and (3.16). This design seeks to keep the state predictions within the region in Ω_{ρ_q} in which $S(q) \le S_{TH}$ when $S(q(t_k)) \le S_{TH}$. This design raises an important point for EMPC in general (i.e., not only LEMPC): if it is desired to enhance process operational safety within EMPC through systems-based safety constraints on the state, it is important for the EMPC to be aware of all dynamics which affect the state (i.e., both those related to the process and those related to equipment) to seek to prevent plant–model mismatch from causing the control actions which an EMPC believes will maintain a process state within a safe operating region from driving the actual process state into unsafe operating regions in state-space. Additionally, it may give greater flexibility to engineers to include the states most heavily tied to a safety issue in $S(q)$, rather than forcing them to develop $S(q)$ from a more limited selection of states which may not be fully capable of assessing safety concerns.

However, the design of Equation (3.31) once again brings to the forefront the need to account for equipment behavior from the beginning of EMPC design. For example, one of the fundamental assumptions of the safety functions of Equation (3.31) is that the state of the system can always be driven back into a neighborhood of the steady-state. Yet, many equipment-related issues (e.g., corrosion) are not reversible, so it is reasonable to postulate that there may be circumstances in which a state used to represent an equipment issue will constantly evolve in an unsafe direction (i.e., it cannot be turned away from this direction) such that if this state is included in $S(q)$ and considered in setting S_{TH}, then once that state causes S_{TH} to be exceeded, the design of Equation (3.31) will not be able to drive $S(q)$ back into the region where $S(q) \leq S_{TH}$. This indicates that to prevent accidents by focusing on the interactions between a process and equipment, new types of safety-based constraints may need to be developed that can constrain potentially irreversible properties (e.g., possibly requiring their values to remain below a certain value in a given time period or to be no worse than under steady-state operation). The safety systems themselves contain equipment that can fail as well, and therefore accounting for potential impacts of the process operating strategy on the ability of equipment comprising the safety system (e.g., burst discs Mannan, 2012) to operate on demand may also improve process operational safety.

In addition, though many EMPC designs apply to the class of systems in Equation (2.1) (i.e., systems of nonlinear ordinary differential equations; there are limited cases where the fundamentally distributed nature of chemical processes has been recognized in EMPC design (Lao *et al.*, 2015a; Lao *et al.*, 2014a; Lao *et al.*, 2014b)), some equipment dynamics (e.g., stress) may need to be modeled using partial differential equations. Due to the fact that equipment may only contact the boundary of a process (e.g., in a reactor, the process conditions which directly affect the reactor vessel are those at the wall of the reactor), it may be necessary to model the process as well with partial differential equations to develop sufficiently accurate predictions of the process conditions at the process–equipment boundary. This may require advances in EMPC theory and formulations. Furthermore, advances in other fields which may benefit control, such as state estimation, may also be required (it may not be possible to measure all states in a control-relevant equipment model; for example, the state z_f in Equation (3.6) is not truly a physical state and therefore it would be expected that state estimation may provide an effective means for obtaining its value). Therefore, output feedback EMPC (Ellis *et al.*, 2014b) for process–equipment systems would also need to be investigated.

Finally, capital cost considerations related to equipment must be considered. EMPC designs focus on profits within a prediction horizon, which have traditionally been assumed to be related to shorter-term operating objectives like reducing energy use or increasing the production rate of a product. The prediction horizon must generally be fairly short to achieve reasonable computation times. However, part of the cost of plant operation is due to maintenance and part replacement as a result of equipment degradation. Therefore, EMPC designs should account for longer-term costs for equipment that may be related to short-term operating conditions (e.g., a penalty can be placed on equipment wear in the objective function) so that the controllers do not make short-sighted decisions that may ultimately reduce the profits of a plant even if they appear to raise them in the short-term. However, accounting for longer-term costs requires that either methods be developed that can account for these longer-term costs in a shorter prediction horizon, or methods dealing with longer prediction horizons in a computationally efficient manner must be developed (Du *et al.*, 2015). Furthermore, with the greater focus on integrating dynamics-related challenges with scheduling to improve operation (Zhuge and Ierapetritou, 2012; Flores-Tlacuahuac and Grossmann, 2010; Tong *et al.*, 2015), scheduling problems should also look at including impacts of the schedule on process equipment (e.g., potentially taking a lead from the literature for cycling of power plants Van den Bergh and Delarue, 2015; Kumar *et al.*, 2012; Hermans and Delarue, 2017; Intertek).

Remark 1. A clarification should be made regarding the relationship between works developed for EMPC to handle equipment (e.g., sensors and actuators) faults or maintenance efforts and the dynamic equipment behavior being proposed for inclusion in EMPC in this work. This can be exemplified by comparing EMPCs accounting for actuator faults (e.g., Alanqar *et al.*, 2017c) and maintenance e.g., Lao *et al.*, 2014c with EMPC accounting for stiction dynamics (Durand and Christofides, 2016). The works which have accounted for actuator faults have assumed $u_a = u_m$, with the result that a fault in the valve would correspond to its unavailability for control (e.g., its output becomes fixed at a specific value until the fault is fixed). In the case where stiction is included, the valve may appear to be stuck at a certain value for some period of time, but that is not because it has experienced a fault. That is a function of its dynamics, which prevent its macroscopic movement until a large enough force is applied to the valve, at which point the valve's dynamics will dictate that it will move (though the results accounting for actuator faults and maintenance should be extended to process–valve systems). Similarly, though sensors may become unavailable due to, for example, maintenance, and their measurements replaced with state estimations until they are brought back on-line (Lao *et al.*, 2015b), this unavailability of the sensor is not due to the dynamic nature of its behavior, but rather due to a physical intervention of maintenance personnel. However, drift in sensor readings over time caused by dynamic effects (potentially, for example, corrosion) would constitute behavior that has the potential to be modeled as part of equipment dynamic behavior of which an EMPC should be made aware.

4

Conclusions

Including valve behavior (e.g., stiction) in EMPC has been demonstrated to be beneficial from the perspective of reducing plant/model mismatch to enable production goals and constraints to be met, and it has been demonstrated that it should be taken into account from the beginning of the design of EMPC formulations to avoid ambiguity in how to handle constraints or practical considerations related to considering the dynamics associated with a process-valve system as opposed to only a chemical process. The benefits of designing EMPCs to account for valve behavior that have been examined in the literature suggest that it may also be desirable to investigate considerations related to other equipment, which may be important from the perspectives of both profit and safety, within EMPC. This review presents the perspective that chemical process systems should be understood not as chemical processes alone, but as being affected by the geometry and dynamics of equipment, and furthermore impacting those equipment dynamics.

Especially with EMPC, which can operate a process in aggressive ways that potentially have more impact on equipment than more traditional MPC designs, it may no longer be adequate to consider equipment selection, design, and materials selection to be design considerations inapplicable to process control strategies.

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