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On accounting for equipment-control interactions in economic model predictive control via process state constraints

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ABSTRACT

Traditionally, chemical processes have been operated at steady-state; however, recent work on economic model predictive control (EMPC) has indicated that some processes may be operated in a more economically-optimal fashion under a time-varying operating policy. It is unclear how time-varying operating policies may impact process equipment, which must be investigated for safety and profit reasons. It has traditionally been considered that constraints on process states can be added to EMPC design to prevent the controller from computing control actions which create problematic operating conditions for process equipment. However, no rigorous investigation has yet been performed to analyze whether, when a process is operated in a time-varying fashion, constraints on the process states (rather than states of the equipment behavior itself) are the most appropriate way of preventing unsafe conditions. In this work, we investigate the use of process state constraints for preventing equipment damage due to the operating conditions set up by an EMPC over time when the equipment behavior is modeled within a context based on forces, deformation, and fracture. Through a chemical process example, we elucidate that there are situations in which process state constraints are likely to be adequate for use in preventing an EMPC from setting up operating conditions that may not be desirable, but that there also may be situations when process state constraints are not adequate and constraints on equipment states may be an alternative. We elucidate a number of challenges that remain to be addressed for this proposed method to be practical.

1. Introduction

EMPC Ellis et al. (2014), Rawlings et al. (2012), Müller et al. (2015), and Huang et al. (2011), Omell and Chmielewski (2013), Jäschke et al. (2014), Liu and Liu (2018) is an optimization-based control design that selects control actions for a process that are economically-optimal, subject to constraints, with respect to a profit metric over a prediction horizon. In many works on EMPC, this profit metric is based on factors such as production rate or the cost of using an input, and may not take its minimum at a process steady-state. The result of this is that EMPC may not operate a process in a fashion that drives the process state to a steady-state, but may instead operate it in a time-varying fashion (i.e., process states such as temperature may vary over time). A strong focus in the EMPC literature has been on the closed-loop stability considerations associated with a control design which can operate processes in a time-varying fashion; this has led to the development of a variety of formulations of EMPC for which closed-loop stability guarantees of various types have been presented (e.g., a terminal cost/constraint formulation (Amrit et al., 2011; Diehl et al., 2011), a formulation with no terminal costs or constraints but with certain assumptions on other aspects of the design such as the prediction horizon length (Grüne, 2013), and a Lyapunov-based constraint formulation (Heidarinejad et al., 2012)). A number of developments have explored practical considerations for EMPC that recognize that equipment

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plays an important role in the effectiveness of the operation of a process under EMPC. For example, Lao et al. (2014) and Lao et al. (2015) develop EMPC designs which can handle actuators and sensors, respectively, being taken off-line for preventive maintenance, and Alanqar et al. (2017) explores a prediction error-triggered approach for identifying actuator faults and subsequently identifying an empirical process model for use in EMPC that adequately captures the process dynamics after the fault. However, these works respond to the impacts of equipment failure on the process state, rather than seeking to investigate how the failure can be predicted or how it may be impacted by the control actions computed by the EMPC. A variety of works have considered equipment degradation or failure at chemical plants when scheduling maintenance protocols (e.g., Wiebe et al., 2018; Vassiliadis and Pistikopoulos, 2001; Dedopoulos and Shah, 1995); however, these do not explicitly unite material dynamics modeling via solid mechanics concepts with EMPC.

The concept that the control actions developed by the EMPC may result in equipment failure is hinted at in Durand et al. (2016), where an EMPC design is developed with input rate-of-change constraints which seek to prevent the EMPC from computing control actions that vary extremely widely between sampling periods, with the motivation for this design being cited as a desire to reduce actuator wear. However, there are many different material failure mechanisms besides wear, such as creep, mechanical and thermal fatigue, and corrosion, which occur due to different molecular-level mechanisms but nonetheless are all impacted by the process operating conditions (e.g., creep is impacted by equipment temperatures due to the process with which the equipment is in contact, mechanical and thermal fatigue are due to variations in mechanical or thermal stresses in equipment over time, and corrosion is caused by chemical reactions between the process constituents and the material from which equipment is constructed). It would be expected, therefore, that a control design that changes the operating conditions over time may cause equipment to fail earlier than it would have under steady-state operation. This is indicated by the literature on time-varying operation for power plants, where power plant cycling has been expected to lead to increased capital and maintenance costs (Lefton et al., 1995). Two important questions with regard to EMPC, therefore, are: (1) whether the control design can be safely utilized (i.e., all potential material failure modes under the control design, for all equipment in the process, can be adequately assessed *a priori* and then an appropriate procedure put in place to perform maintenance or equipment replacement before the material fails by any such mechanism); (2) whether EMPC remains economically attractive when the potential for increased capital and maintenance costs are accounted for in the analysis of the total profit.

With regard to safe use of EMPC, a number of recent works (e.g., Albalawi et al., 2017a,b; Wu et al., 2018) have explored the use of explicit safety constraints in EMPC that are based on the location of the process state in state-space. Though it has been recognized that these could be applied in cases where the equipment dynamics are modeled such that there are states for the equipment that can be constrained to prevent safety issues (Durand and Christofides, 2018), no in-depth discussion of how such constraints can be developed has been presented. One idea for analyzing profits when both instantaneous operating costs as well as capital (Etoughe et al., 2018) and maintenance costs are accounted for would be, inspired by the work on integrated design and control (Chawankul et al., 2007; Patel et al., 2008; Sakizlis et al., 2004), to attempt to develop a profit metric for use as the stage cost of an EMPC that reflects total plant profit, including the operating costs/profit as well as capital equipment costs. This would require a mapping to be made between operating conditions such as temperature and pressure and equipment costs. A potentially more straightforward method that could also have benefits from a process operational safety standpoint would be to recognize that the capital/maintenance equipment costs depend on material degradation, where modeling of both the process and material/equipment behavior could allow the material degradation to be predicted by the EMPC as a function of the operating conditions it sets up. The goal would then be to develop appropriate constraints for the EMPC that force it to compute control actions which would prevent material failure but are economically-optimal with respect to profit metrics based on instantaneous operating costs/profit subject to such a constraint. This line of thinking (i.e., developing models for use in EMPC that reflect the coupling between process and equipment states) has many similarities to the thinking presented in Durand and Christofides (2016) for handling friction in valves (valve stiction), where due to the fact that coupling between the controller, process, and valve dynamics causes problematic behavior in control loops containing sticky-valves (e.g., poor set-point tracking) (Durand et al., 2018), a strategy for compensating for valve behavior that uses the process-valve model in model predictive control design was proposed so that the controller would be aware of the coupling when computing control actions and compute appropriate control actions in light of this.

In this work, we provide initial steps in the direction of investigating equipment-control interactions for processes operated under EMPC by considering the traditional method for accounting for equipment fidelity in model predictive control, which is to place state constraints on the process states and to thereby constrain some aspect of the equipment behavior, but to avoid modeling the equipment behavior explicitly. Through a simple yet illustrative chemical process example, we explore a type of material behavior which might be constrained by process state constraints, rather than equipment constraints. We demonstrate that while there are many considerations which may be captured by such constraints, time-varying operation may set up equipment conditions outside of the types of material behavior which are normally modeled, and attempting to account for these with process state constraints may lead to unnecessary conservatism in the control design. We propose that an alternative method for accounting for equipment-control interactions would be to incorporate dynamic models of equipment behavior within EMPC design; however, we also demonstrate that this is a challenging task, with many unanswered questions of which we seek to present a subset for the purpose of spurring further research in this area. This work is an extended version of Durand (2019).

2. Preliminaries

2.1. Notation

The Euclidean norm of a vector is denoted by $|\cdot|$. A class $\mathcal{K}$ function $\alpha : [0, a) \to [0, \infty)$ is strictly increasing with $\alpha(0) = 0$. The transpose of a vector x is denoted by x^T. Set subtraction is signified by "/" such that $x \in A/B := \{x \in R^n : x \in A, x \notin B\}$. A level set of a positive definite function V is denoted by $\Omega_\rho := \{x \in R^n : V(x) \le \rho\}$. R_+ signifies the set of non-negative real numbers.

2.2. *Class of systems*

In this work, we focus on chemical process systems that can be described by systems of ordinary differential equations of the following form:

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

where f is a locally Lipschitz nonlinear vector function, $x \in X \in R^n$ is the state vector, $u \in U \subset R^m$ is the vector of manipulated inputs, and $w \in W \subset R^z$ is the vector of bounded disturbances ($W := \{w \in R^z : |w| \le \theta\}$). We consider that $f(0, 0, 0) = 0$ (the origin is an equilibrium of the system of Eq. (1)). We furthermore assume that the system of Eq. (1) is stabilizable in the sense that there exists a sufficiently smooth positive definite Lyapunov function $V : R^n \to R_+$, functions $\alpha_j(\cdot)$, $j = 1, \ldots, 4$, of class $\mathcal{K}$, and a controller $h_1(x)$ that can asymptotically stabilize the origin of the closed-loop system of Eq. (1) in the absence of disturbances such that the following inequalities are satisfied:

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

$$\frac{\partial V(x)}{\partial x} f(x, h_1(x), 0) \le -\alpha_3(|x|) \tag{3}$$

$$\left|\frac{\partial V(x)}{\partial x}\right| \le \alpha_4(|x|) \tag{4}$$

$$h_1(x) \in U \tag{5}$$

for all $x \in D \subset R^n$, where D is an open neighborhood of the origin. We call a level set $\Omega_\rho \subset D \cap X$ of V the stability region.

2.3. *Economic model predictive control*

EMPC is a control design for which the inputs are computed via the following optimization problem:

$$\min_{u(t) \in S(\Delta)} \int_{t_k}^{t_{k+N}} L_e(\tilde{x}(\tau), u(\tau))\, d\tau \tag{6a}$$

$$\text{s.t.} \quad \dot{\tilde{x}}(t) = f(\tilde{x}(t), u(t), 0) \tag{6b}$$

$$\tilde{x}(t_k) = x(t_k) \tag{6c}$$

$$\tilde{x}(t) \in X, \ \forall\, t \in [t_k, t_{k+N}) \tag{6d}$$

$$u(t) \in U, \quad \forall\, t \in [t_k, t_{k+N}) \tag{6e}$$

where $u(t)$ is a piecewise-constant input vector trajectory with N pieces (N is the prediction horizon), where each piece is held for a period Δ (i.e., $u(t) \in S(\Delta)$). The economics-based stage cost L_e of Eq. (6) need not have its minimum at a process steady-state. It is evaluated throughout the prediction horizon using predictions $\tilde{x}$ of the process state from the model of Eq. (6b) (i.e., the model of Eq. (1) without disturbances) initialized from the state measurement at t_k (i.e., Eq. (6c)). The constraints of Eqs. (6d) and (6e) are state and input constraints, respectively. The first of the N pieces of the input vector trajectory that is the optimal solution to the optimization problem is applied to the process (i.e., a receding horizon implementation is employed). The optimal solution at t_k is denoted by $u^*(t_i|t_k)$, where $i = k, \ldots, k+N$. EMPC with a quadratic objective function that takes its minimum at the process steady-state (i.e., $L_e = x^T Q\, x + u^T R\, u$, with Q and R as positive definite matrices) has been utilized extensively in the process industries (Qin and Badgwell, 2003) and is often referred to as model predictive control (MPC) or tracking MPC.

A specific formulation of EMPC with two Lyapunov-based stability constraints added to the EMPC formulation in Eq. (6) is known as Lyapunov-based EMPC (LEMPC). The formulation of these two added constraints is as follows (Heidarinejad et al., 2012):

$$V(\tilde{x}(t)) \le \rho_e, \quad \forall\, t \in [t_k, t_{k+N}), \quad \text{if} \ \ x(t_k) \in \Omega_{\rho_e} \tag{7a}$$

$$\frac{\partial V(x(t_k))}{\partial x} f(x(t_k), u(t_k), 0) \le \frac{\partial V(x(t_k))}{\partial x} f(x(t_k), h_1(x(t_k)), 0) \quad \text{if} \ \ x(t_k) \in \Omega_\rho / \Omega_{\rho_e} \tag{7b}$$

where $\Omega_{\rho_e} \subset \Omega_\rho$ is a subset of the stability region that makes Ω_ρ forward invariant under the controller of Eqs. (6) and (7).

3. Accounting for equipment-control interactions in EMPC design via process state constraints

Industrial implementations of tracking MPC utilize a process dynamic model in Eq. (6b) that is based on the dynamics of the process only (not equipment). Inspired by recent work on including valve dynamics in EMPC (Durand and Christofides, 2016), it has been suggested that equipment behavior might be accounted for by incorporating process-equipment models in EMPC and appropriately constraining the equipment states (Durand and Christofides, 2018). However, this would add additional dynamic states to the model of Eq. (6b), increasing the time required to solve this dynamic system. Traditionally, the constraint of Eq. (6d) is considered to already include any constraints which might be developed for equipment purposes (e.g., a constraint on the temperature in a reactor might be considered to prevent damage of the reactor equipment). It is therefore desirable to investigate how well these constraints can constrain material behavior, to better understand the conditions under which equipment behavior might need to be modeled and constrained, with greater computational effort, instead of taking advantage of the constraints of Eq. (6d) that do not require additional dynamic models to be developed and solved.

To begin this investigation, we consider a simple yet illustrative chemical process consisting of a continuous stirred tank reactor (CSTR) controlled by an EMPC, and followed by a section of process piping which is heated by the process fluid exiting the CSTR beyond the steady-state temperature it was designed for. For this case, we associate a model with the pipe material behavior to investigate the impact of the EMPC's actions on this piece of equipment.

3.1. *Illustrative example: EMPC and equipment-control interactions*

Though the CSTR under consideration has been examined in a number of works (e.g., Heidarinejad et al., 2012; Albalawi

Table 1 – Parameters for the CSTR model.

Parameter	Value	Unit
V	1	m^3
T_0	300	K
C_p	0.231	kJ/kg·K
k_0	8.46×10^6	m^3/h kmol
F	5	m^3/h
ρ_L	1000	kg/m^3
E	5×10^4	kJ/kmol
R_g	8.314	kJ/kmol K
ΔH	-1.15×10^4	kJ/kmol

et al., 2017b; Alanqar et al., 2015), it is necessary to consider how to appropriately model the pipe material. Fundamentally, the impacts of operating conditions on equipment material fidelity are driven by molecular mechanisms. It is common in mechanical design to seek to represent these molecular-level phenomena by aggregate solid material behavior via the notions of solid mechanics (this is similar to the sense in which the molecular-level phenomena in fluid flow are often represented in the aggregate by the equations of fluid mechanics). In this initial example, we utilize the principles of solid mechanics (which are based on force balances within infinitesimally small volumes of a solid coupled with fits of material testing data to mathematical expressions which due to their data-fitting derivation, come with some uncertainty) to describe the behavior of the pipe material. However, we will subsequently discuss some of the limitations of force and deformation-based analyses for handling phenomena that could be expected when time-varying operation is considered.

The piping element is considered to follow closely after the reactor such that the fluid temperature is considered to be the same at the entrance to this pipe as it is in the outflow of the CSTR. This pipe is considered to be rigidly fixed at one end with a bellows joint on the other and is insulated. The pipe is assumed to have negligible impact on the mixing in the tank, and its dimensions and properties are taken from Barron and Barron (2012). Specifically, the pipe has an inner radius of 0.05115 m, an outer radius of 0.05715 m, and a length L of 2.54 m. It is made of an alloy with an ultimate strength of 400 MPa, a yield strength of 270 MPa, a Young's Modulus of 200 GPa, and a thermal expansion coefficient of 12.5×10^{-6} K^{-1}.

Within the CSTR, the exothermic second-order reaction $A \rightarrow B$ occurs. The manipulated inputs for the CSTR are the concentration C_{A0} of the reactant in the feed and the heat rate Q which can be added or removed by a heating/cooling jacket. The dynamics of the process are as follows, with process parameters listed in Table 1:

$$\dot{C}_A = \frac{F}{V}(C_{A0} - C_A) - k_0 e^{-\frac{E}{R_g T}} C_A^2 \tag{8}$$

$$\dot{T} = \frac{F}{V}(T_0 - T) - \frac{\Delta H k_0}{\rho_L C_p} e^{-\frac{E}{R_g T}} C_A^2 + \frac{Q}{\rho_L C_p V} \tag{9}$$

where C_A and T are the state variables representing the reactant concentration and temperature in the reactor over time, R_g is the ideal gas constant, E is the reaction activation energy, ΔH is the enthalpy of reaction, and k_0 is the pre-exponential constant. The inlet/outlet volumetric flow rate F is considered fixed, as are the liquid density ρ_L, heat capacity C_p, and liquid volume V. Vectors of deviation variables for the states C_A and T and inputs C_{A0} and Q from their steady-state values $C_{As} = 1.22$ kmol/m^3, $T_s = 438.2$ K, $C_{A0s} = 4$ kmol/m^3, and $Q_s = 0$ kJ/h, respectively, are $x = [x_1\ x_2]^T = [C_A - C_{As}\ T - T_s]^T$ and $u = [u_1\ u_2]^T = [C_{A0} - C_{A0s}\ Q - Q_s]^T$.

Though the velocity of the fluid through the outlet pipe does not change over time (F is constant), its temperature changes due to changes in the inputs C_{A0} and Q over time as computed by the EMPC. Specifically, the EMPC adjusts C_{A0} and Q, affecting T, in a manner that seeks to optimize the production rate of the desired product as follows:

$$L_e = -k_0 e^{-\frac{E}{R_g T(\tau)}} C_A(\tau)^2 \tag{10}$$

Input constraints are also enforced in the EMPC optimization problem requiring that $0.5 \leq C_{A0} \leq 7.5$ kmol/m^3 and $-5 \times 10^5 \leq Q \leq 5 \times 10^5$ kJ/h.

Furthermore, Lyapunov-based stability constraints of the form in Eq. (7) are imposed (the constraint of Eq. (7a) was enforced at the end of each sampling period when $x(t_k) \in \Omega_{\rho_e}$ and also at the end of every sampling period after the first when $x(t_k) \in \Omega_\rho / \Omega_{\rho_e}$ to constrain the state after t_k). These Lyapunov-based stability constraints are developed using $V = x^T P x$, where $P = [1200\ 5\ ;\ 5\ 0.1]$. The Lyapunov-based control law $h_1(x)$ was developed such that its first component $h_{1,1}(x)$ was fixed at 0 kmol/m^3 for simplicity, whereas its second component $h_{1,2}(x)$ was computed via Sontag's control law (Lin and Sontag, 1991) as follows:

$$h_{1,2}(x) = \begin{cases} -\dfrac{L_{\tilde{f}}V + \sqrt{L_{\tilde{f}}V^2 + L_{\tilde{g}_2}V^4}}{L_{\tilde{g}_2}V}, & \text{if } L_{\tilde{g}_2}V \neq 0 \\ 0, & \text{if } L_{\tilde{g}_2}V = 0 \end{cases} \tag{11}$$

but with the value of $h_{1,2}(x)$ from Eq. (11) saturated at its bounds if these bounds were reached. $\tilde{f}$ in Eq. (11) represents the vector-valued function that is not related to the inputs in the deviation variable form of Eqs. (8)-(9), and $\tilde{g}$ represents the matrix-valued function that multiplies the input vector in the deviation variable form of the process model equations ($\tilde{g}_2$ represents its second column). $L_{\tilde{f}}V$ and $L_{\tilde{g}_2}V$ represent the Lie derivatives of V with respect to $\tilde{f}$ and $\tilde{g}_2$. Using a discretization of the state-space between $C_A = 0$ kmol/m^3 and 4 kmol/m^3 and between $T = 340$ K and 560 K, where the concentration intervals were 0.01 kmol/m^3 and the temperature intervals were 1 K, $\rho = 300$ was selected so that the value of T was able to become significantly larger than the steady-state value within the allowable operating region Ω_ρ (for the purpose of the thermal strain analyses to be presented below). ρ_e was arbitrarily set to 75% of ρ. The process state was initialized from $x_{init} = [-0.4\ \text{kmol/m}^3\quad 8\ \text{K}]^T$, N was set to 10, and Δ was set to 0.01 h. An integration step of 10^{-4} h was utilized to simulate the process, and was also used to make the state predictions within the EMPC. The simulations were performed for one hour of operation using MATLAB and the function fmincon. In the optimization problem, the value of u_2 was scaled down by 10^5 to account for the large magnitude of this term, and the initial guess for the decision variables was the steady-state values of the inputs at each sampling time. The optimization problem was feasible in all sampling periods.

The trajectories of the states and inputs throughout the one hour of operation are depicted in Figs. 1 and 2 . As shown in Fig. 1, the temperature of the stream leaving the CSTR increases to approximately 490.2 K and remains there there-

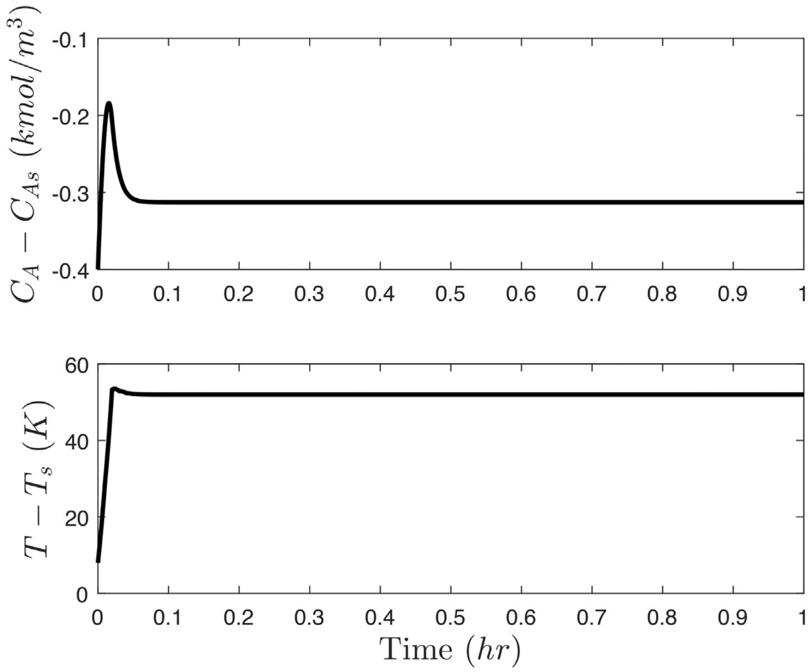

Fig. 1 – States over one hour of operation for the process of Eqs. (8)–(9) under the EMPC that does not account for limitations on u_1.

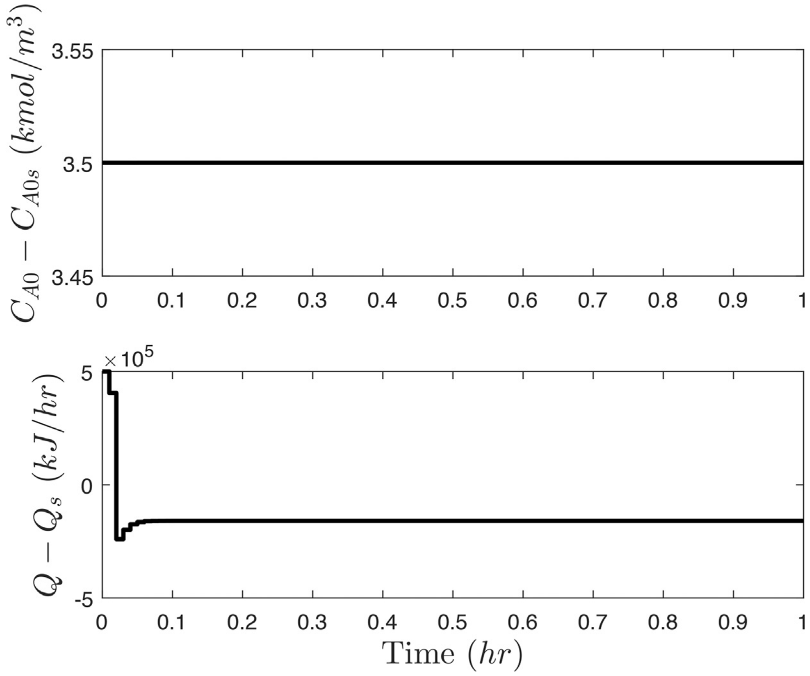

Fig. 2 – Inputs over one hour of operation for the process of Eqs. (8)–(9) under the EMPC that does not account for limitations on u_1.

after. This indicates that the temperature of the insulated pipe downstream of the CSTR, through which the fluid is flowing at approximately 490.2 K, should eventually reach 490.2 K as well after sufficient time passes, if the EMPC was to continue to operate the process at 490.2 K. To examine how a constraint with the form in Eq. (6d) might be developed that is explicitly related to equipment limitations, we will explore the thermal stresses in the pipe when it reaches this new temperature and compare them with the thermal stresses for steady-state operation (i.e., $T = 438.2$ K).

We consider that the stresses in the pipe are only in the axial direction and that they result from the constraints on the ends of the pipe (we neglect any edge effects at the pipe ends or any effects from the insulation on the radial thermal expansion, and assume that the radial thermal expansion occurs freely such that it is only the axial expansion that experiences constraints). Furthermore, we assume that we will operate the process in a manner where the stress remains less than the elastic limit. The strain ϵ (i.e., material deformation, or the fractional change in length of a material compared to its original length) is typically considered to be induced by both temperature T (i.e., thermal expansion) and stress σ (i.e., the force on a solid per unit area). Assuming that the material has a proportional relationship between differential changes in stress and strain below the elastic limit equal to the Young's modulus E (i.e., $E = \left(\frac{\partial \sigma}{\partial \epsilon}\right)_T$), that E and the thermal expansion coefficient for linear thermal expansion in the axial direction α can be approximated as constant in the range of operating conditions considered, and that the zero-strain condition is at $T = 293.15$ K, the following equation relates stress and strain in the pipe after the temperature of the pipe has reached T_f uniformly throughout (Barron and Barron, 2012):

$$\sigma = E\epsilon - \alpha E(T_f - 293.15) \tag{12}$$

where all terms are in SI units (e.g., T_f is in K). This is an equilibrium relationship and therefore this does not capture the time-dependence of stress/strain as the pipe is heated (which would be desirable to capture from a control point of view, as control is based on dynamic behavior); however, as will be shown below, the fact that it considers an equilibrium situation allows the condition to be used in defining a state constraint of the form in Eq. (6d) for the EMPC under consideration.

To see how such a constraint might be developed, we first explore how the EMPC's control action decisions, when implemented without the EMPC being aware of the equipment material limitations, might impact the stress/strain in the pipe. To analyze this, we utilize the analysis techniques for computing equilibrium compressive stress in a pipe at elevated temperature for various pipe equipment constructions from Barron and Barron (2012). After sufficient time has passed so that the pipe temperature has reached equilibrium under the control actions computed by the EMPC, $T_f = 490.2$ K. When the pipe is at 293.15 K (i.e., it has not experienced thermal strain), the force from the stress on the pipe is equal to the force on the pipe from the bellows joint (modeled like a spring force with spring constant k_s), with the result that the stress in the pipe is given by (Barron and Barron, 2012):

$$\sigma = \frac{-\alpha E(T_f - 293.15)}{1 + \frac{AE}{k_s L}} \tag{13}$$

where A is the area of the pipe in contact with the wall/bellows joint ($A = 0.002041\ \mathrm{m}^2$) and a negative stress indicates a compressive stress. By adjusting the stiffness of the bellows joint (i.e., different values of k_s), we can find conditions under which the equipment fidelity may be compromised (which aids in developing appropriate equipment-based constraints for the EMPC). We first will consider an extreme case in which we see what would happen if the value of k_s was set assuming a steady-state operating policy and assuming that the maximum temperature that might be reached in the pipe is 10 K above the steady-state value (i.e., 448.2 K). In that case, the maximum value of k_s according to Eq. (13) that would be needed to ensure that the stress was no greater than a design value of 10^8 Pa (which is less than the yield strength) at a high-temperature equilibrium condition would be 5.58×10^7 N/m. Therefore, we consider a case where the spring constant utilized is 5.50×10^7 N/m, which is less than the maximum value and therefore would be expected under the hypothetical steady-state operating scenario where the temperature is not expected to exceed 448.2 K to maintain the stress below the desired 10^8 Pa threshold. However, if this bellows joint is used and the control design for the process with this spring constant is changed from a controller enforcing steady-state operation around the steady-state with $T_s = 438.2$ K to the EMPC that operates the process as shown in Fig. 1, the stress in the pipe when the temperature throughout the pipe reaches 490.2 K becomes 1.26×10^8 Pa, which is above the desired threshold. Alternatively, if the spring constant for the bellows is much lower (e.g., $k_s = 4.4 \times 10^5$ N/m, which Barron and Barron (2012) cites as a more typical spring constant for a bellows such that this scenario is expected to be more realistic), then even the higher temperatures reached under the operation with the EMPC are unlikely to cause the stress to reach a high level (in this example, the equilibrium stress when $k_s = 4.4 \times 10^5$ N/m and $T_f = 490.2$ K would be 1.34×10^6 Pa, which is significantly lower than the 10^8 Pa threshold).

Returning to the extreme case with $k_s = 5.50 \times 10^7$ N/m for the sake of illustration, we can consider preventing the thermal stress from exceeding the design value at an equilibrium condition where the temperature remains constant for an extended period of time using a constraint of the form in Eq. (6d) (i.e., we would like to develop a constraint on one of the states of the process dynamic model, but to have this constraint on a process state avoid an undesirable condition at the equipment level). From a physics perspective, the goal is to constrain the stress in the pipe via the EMPC. At the equilibrium condition expressed by Eq. (13), the value of T_f is considered to be the same as the value of T. Therefore, if we constrain the equilibrium compressive stress (requiring $\sigma > -10^8$ Pa, $\forall t \in [t_k, t_{k+N})$ in the EMPC), we could rewrite the resulting equation as a bound on the temperature out of the CSTR (i.e., $T < 450$ K). This constraint ensures that the temperature of the fluid in the pipe never reaches a value where, if an equilibrium condition were set up in the pipe at any time, the temperature in that pipe at the equilibrium could be greater than the temperature which would cause the stress in the pipe to exceed the design value.

The results for a simulation of the CSTR process under the LEMPC described above but with the constraint $T < 450$ K added as a state constraint are shown in Fig. 3, where the new state constraints on T are enforced at every integration step, and the constraint requiring $V(\tilde{x}) \le \rho_e$ is also enforced at the end of every integration step both when Eq. (7a) is used and when Eq. (7b) is used. The optimization problem was feasible at each sampling time. The inputs which create the oscillatory behavior in T toward the beginning of the time of operation also generate a higher profit than would be obtained in that time period by using a constant value of C_{A0} and a constant value of Q that approximate the values that are reached for the majority of the time of operation in Fig. 4, but while still meeting the state and stability constraints as reflected in Figs. 3 and 5 . We see that an equilibrium condition is set up once again, with the result that the assumption of equilibrium used in developing the constraint remains useful. The time-averaged value of the stage cost of Eq. (10) over the hour of operation is 13.88 for operation at the steady-state, 32.85 for the EMPC in Fig. 1, and 29.40 for the EMPC in Fig. 3.

An alternative to enforcing a hard constraint on temperature in the LEMPC would be to find a stability region in which the value of T does not exceed 450 K and to then modify the LEMPC to include Lyapunov-based stability constraints based on this new stability region. The reason that this might be explored instead of the hard constraint utilized in the simulation above is that from a theoretical perspective, no closed-loop stability or recursive feasibility guarantees can be made for LEMPC with a general hard constraint that is not satisfied everywhere in Ω_ρ. By restricting Ω_ρ to be contained within the region where $T < 450$ K, it would be possible to theoretically guarantee that the closed-loop state will always remain in the region where $T < 450$ K under sufficient con-

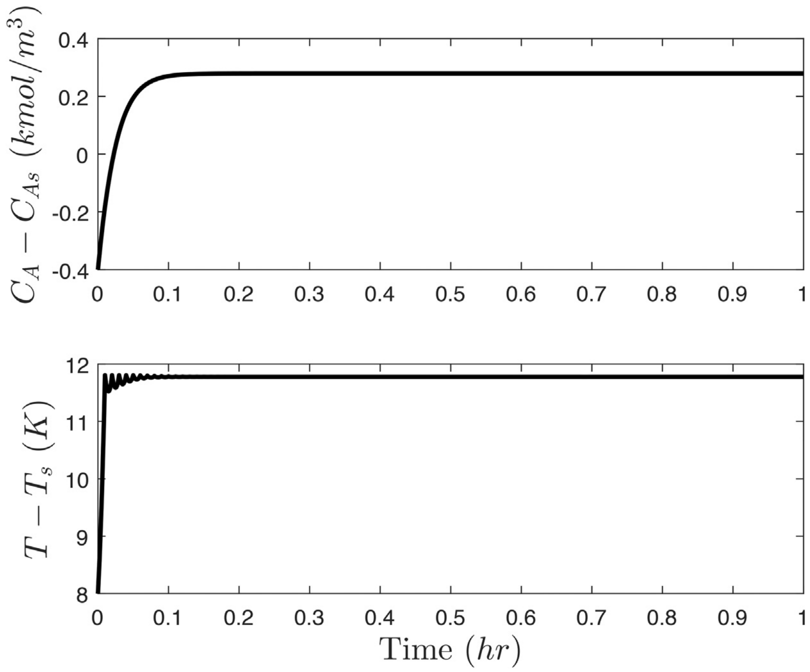

Fig. 3 – States over one hour of operation for the process of Eqs. (8)–(9) under the EMPC with a hard constraint on T.

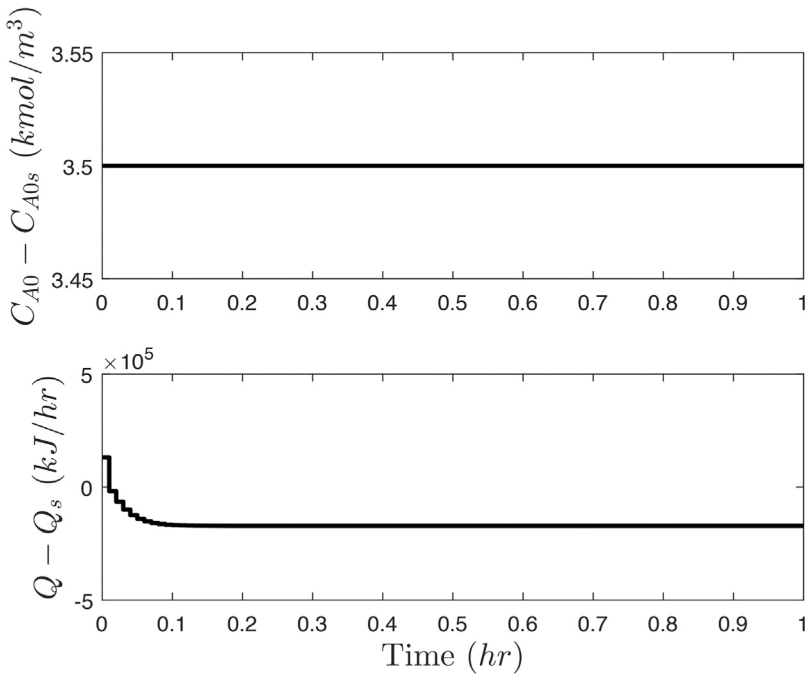

Fig. 4 – Inputs over one hour of operation for the process of Eqs. (8)–(9) under the EMPC with a hard constraint on T.

ditions (Heidarinejad et al., 2012). However, this would be expected to require that the closed-loop state remain in a smaller region of operation than it is restricted to with the hard constraint, and as a result would be expected to negatively impact profits, just as the restriction on T reduced the profit of the EMPC in Fig. 3 compared to the EMPC in Fig. 1.

In the EMPC design for Fig. 1, the EMPC essentially drove the closed-loop state to a more profitable steady-state that was not the operating steady-state. Though it could be argued that this is reasonable behavior as compared to operating at the other steady-state because the region Ω_ρ is the region we want to operate in rather than a different set of allowable operating conditions around the higher-temperature steady-state, we can also explore a case where the connection to the steady-state with $u_1 = 0\,\text{kmol/m}^3$ is more explicit. In this case, we consider the same process as above except that we consider that we would like the time-averaged amount of reactant fed to the reactor in every hour of operation to be as close as possible to that which would be fed at steady-state, meaning that we would like the following equation to be satisfied as closely as possible:

$$\frac{1}{1\ \text{h}} \int_{t=0\ \text{h}}^{t=1\ \text{h}} u_1(\tau)d\tau = 0\ \ \text{kmol/m}^3 \tag{14}$$

This constraint prevents the EMPC from driving the closed-loop state to a new operating condition and thereafter maintaining it at such a condition. For this simulation, because the constraint of Eq. (14) is not guaranteed to be satisfied, it was implemented with slack variables to ensure

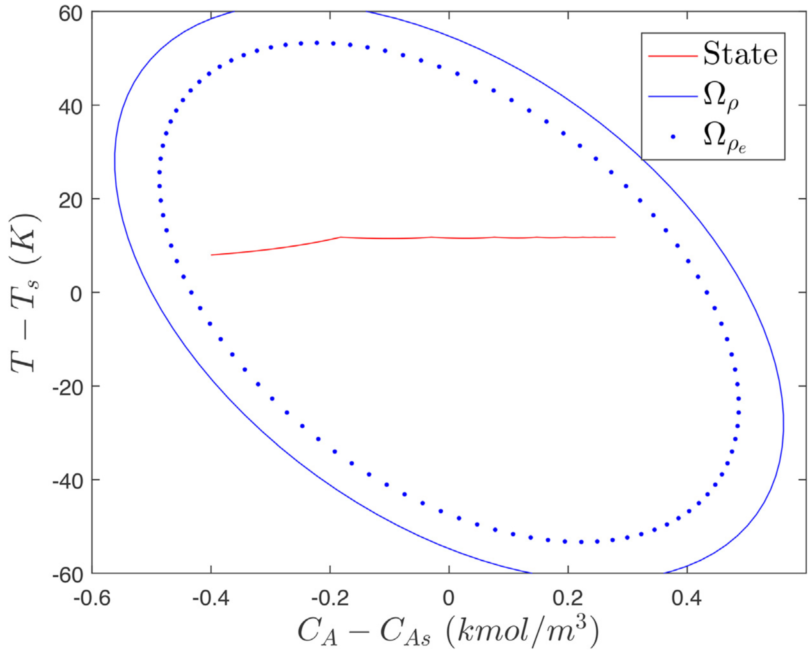

Fig. 5 – State-space trajectories over one hour of operation for the process of Eqs. (8)–(9) under the EMPC with a hard constraint on *T*.

feasibility of the optimization problem at every sampling time, which resulted in the time-averaged value of u_1 being equal to 0.4007 kmol/m^3 in the first hour (this is much closer to the desired value of 0 kmol/m^3 than what would be achieved in the case in Fig. 1 without the constraint on the input, where the time-averaged value of u_1 reaches 3.5 kmol/m^3). Specifically, the constraint was implemented in the manner described in Ellis et al. (2014) but with slack variables s_1 and s_2 as follows:

$$s_1 \geq \sum_{i=0}^{k-1}(u_1^*(t_i|t_i)) + \sum_{i=k}^{k+N_k}(u_1(t_i|t_k)) - 3.5\delta\left(100 - \frac{t_k}{\Delta} - N\right) \tag{15}$$

$$s_2 \geq -\sum_{i=0}^{k-1}(u_1^*(t_i|t_i)) - \sum_{i=k}^{k+N_k}(u_1(t_i|t_k)) - 3.5\delta\left(100 - \frac{t_k}{\Delta} - N\right) \tag{16}$$

where $N_k = N$ and $\delta = 1$ for $t_k < 0.9$ h, and $\delta = 0$ and N_k is set to the number of sampling periods remaining in the operating period of 1 h when $t_k \geq 0.9$ h. Fig. 6 shows the states in this case. The guess of the slack variables provided to the optimization solver was 0 at each sampling time, and they were effectively unbounded in the optimization problem (the upper and lower bounds of s_1 and s_2 were 2×10^{19} and -2×10^{19}, respectively). The objective function minimized in this case with the slack variables was as follows:

$$\int_{t_k}^{t_{k+N}} \left[-k_0 e^{-\frac{E}{R_g T(\tau)}} C_A(\tau)^2\right] d\tau + 100(s_1^2 + s_2^2) \tag{17}$$

The coefficient of 100 for the slack variable term was chosen in a relatively *ad hoc*/trial-and-error fashion with the goal of seeking to avoid reducing the profit too much by causing it to compete with the slack variable term, while simultaneously seeking to drive the slack variables toward zero to avoid violations of the constraint in Eq. (14) in a feasible manner.

Figs. 6-7 show the state and input trajectories under the EMPC accounting for the added constraints in Eqs. (15)-(16) and the modified objective function of Eq. (17). In Fig. 6, the value of T increases again to around 490 K and remains there for some time. This indicates that there may be EMPC cases for the process under consideration where, depending on the heat transfer coefficient and thermal conductivity for the pipe, considerations like equilibrium stress could be relevant, even if the process state is not fixed at that condition permanently. This is seen to potentially be relevant by analyzing the speed with which the temperature in the pipe is expected to change in response to a change in the temperature of the fluid leaving the CSTR. Specifically, consider the case in Fig. 6, where without any constraint on the temperature, the temperature of the fluid leaving the CSTR reaches the temperature of about 490.2 K for only a short period of time (about 0.4 h). Neglecting axial variations in temperature in the pipe for simplicity for the purpose of understanding the approximate speed with which the temperature changes throughout the pipe, we model the heat conduction through the pipe wall via the following partial differential equation:

$$\frac{\partial T_p}{\partial t} = \alpha_c \frac{\partial^2 T_p}{\partial x_{space}^2} \tag{18}$$

where x_{space} refers to the spatial coordinate (i.e., $x_{space} = 0$ m refers to the inner wall of the pipe, and $x_{space} = 0.006$ m refers to the outer wall of the pipe), $T_p(x_{space}, t)$ refers to the temperature in the pipe as a function of time and space, and α_c represents the thermal diffusivity (taken to be 1.163×10^{-5} m^2/s based on values of the thermal conductivity, density, and heat capacity of AISI 4140 alloy steel Bohler Uddeholm Australia). The boundary and initial conditions are considered to be as follows:

$$\frac{\partial T_p}{\partial x_{space}}(x_{space} = 0 \quad \text{m}, t) = \frac{h_{tc}}{k}(T - T_p) \tag{19}$$

$$\frac{\partial T_p}{\partial x_{space}}(x_{space} = 0.006 \quad \text{m}, t) = 0 \tag{20}$$

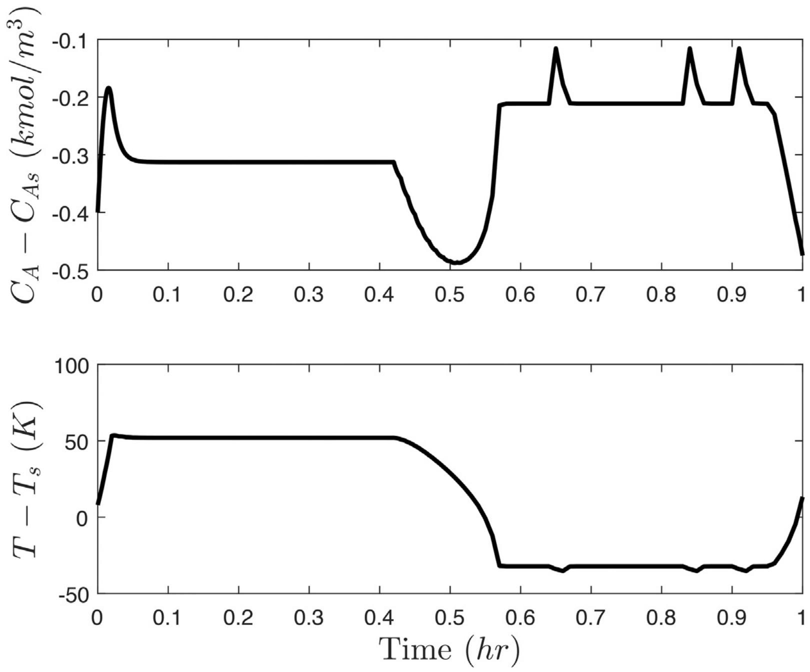

Fig. 6 – States over one hour of operation for the process of Eqs. (8)–(9) under EMPC with the slack variables in the constraints of Eqs. (15)–(16).

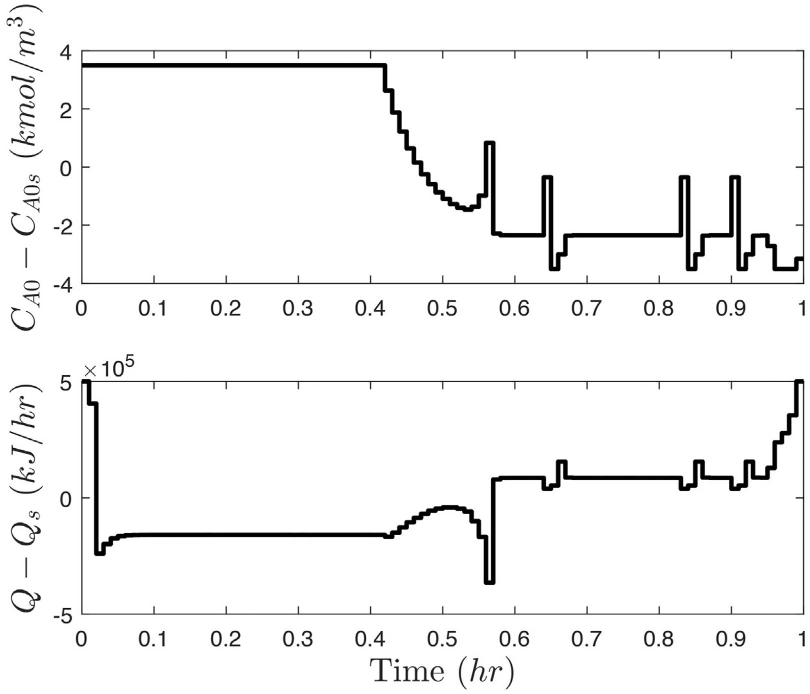

Fig. 7 – Inputs over one hour of operation for the process of Eqs. (8)–(9) under EMPC with the slack variables in the constraints of Eqs. (15)–(16).

$$T_p(x_{space}, t = 0\ \ s) = 438.2\ \ K \tag{21}$$

where the boundary condition in Eq. (19) reflects that heat is transferred from the process fluid to the process piping (i.e., there is coupling between the process and equipment states), Eq. (20) reflects that the pipe is insulated, and Eq. (21) reflects that the pipe is considered to be at the temperature corresponding to the steady-state outlet temperature of the CSTR before the inner pipe wall is brought to 490.2 K at t = 0 s (reflecting an approximation of a negligible transient in the value of T in the pipe for the purpose of gaining an understanding of the order of magnitude of time that it takes for the pipe material to respond to temperature changes in the fluid flowing from the CSTR). Simulating this pipe with the method of lines using 20 interior nodes for the spatial finite differences and two fictitious nodes in implementing the boundary conditions and an integration step of 10^{-3} s in computing the temporal variation in the resulting 22 state variables, with the heat transfer coefficient h_{tc} for the fluid-solid heat transfer phenomenon (taken to be 3000 W/m^2 K) and the thermal conductivity k of the solid (set to 42 W/m K based on the value reported for 4140 steel in Bohler Uddeholm Australia), the results in Fig. 8 were obtained. From this figure, it is seen that heat conduction through the pipe is fairly rapid upon a temperature

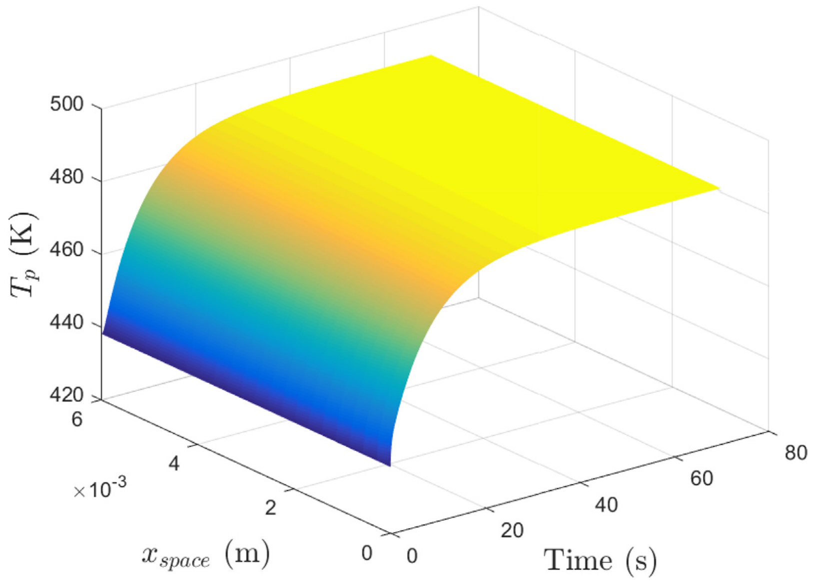

Fig. 8 – Heat conduction through the pipe in one dimension, assuming that the heat transfer resistance at the inner pipe wall is taken into account via Eq. (19).

change in the fluid in the pipe, particularly compared to the timescale over which the EMPC keeps the pipe temperature at a fixed value in Fig. 6. In cases where the behavior of the EMPC without constraints on the process states may be like this, equilibrium considerations may play an important role in the design of constraints for an EMPC that is attempting to explicitly account for material behavior to avoid allowing such equilibrium conditions to be set up.

Remark 1. Though the constraint added to the EMPC in Fig. 3 is a state constraint, it should be noted that it is not actually the process state which we desire to constrain, but rather the temperature within the pipe material itself (a state of the equipment rather than a state of the process). For the case presented above, this can be reformulated as a constraint on the process state. In cases such as this where the equipment considerations can be reformulated as state constraints on process states and the EMPC is of the form of Eqs. (6) and (7) with these added state constraints, the closed-loop stability results for an EMPC of this form that have been previously developed (Heidarinejad et al., 2012) can be utilized. Specifically, such a state constraint could be handled with stability and feasibility guarantees by changing ρ such that Ω_ρ is contained only within the region where the new state constraint (e.g., the bound on *T*) is satisfied. If a hard constraint is instead added to the EMPC, recursive feasibility and closed-loop stability are not guaranteed, but as in Albalawi et al. (2017b), a backup control law could be utilized if the control law is infeasible. However, as stated in Albalawi et al. (2017b), the resulting EMPC-backup control law combination would not be guaranteed to maintain the closed-loop state in the region where the state constraint was met (which as in the case described above might result in the thermal stress in the pipe exceeding the desired value), though it could maintain it in Ω_ρ.

Remark 2. It is not required that Lyapunov-based stability constraints be utilized in an EMPC that accounts for equipment behavior via a process state constraint (Rawlings et al., 2012). A benefit of the use of such constraints when examining equipment considerations, however, is that they provide an explicitly characterizable (*a priori*) region in state-space within which the process state will remain under sufficient conditions. When the constraints related to materials can be expressed as process state constraints as in this example, it is beneficial to be able to ensure, *a priori*, that under the sufficient conditions, the closed-loop state of the process will never reach values that could compromise the equipment (at least for the failure mechanisms being considered), as that would pose a safety hazard that must be avoided under EMPC.

4. Challenges with accounting for equipment-control interactions in EMPC via process state constraints

The example in the above section suggests that process state constraints of the form in Eq. (6d) can be adequate for constraining some types of material behavior, and particularly some of those which are associated with an equilibrium condition. However, the transients in the simulations in Figs. 3 and 6 are a reminder that the approach which we have taken so far to handling equipment-control interactions in EMPC design may not be able to account for types of material behavior that are not adequately represented through equilibrium relationships. Because EMPC may operate processes with time variations in process states, it may not always cause equilibrium stress conditions to hold. The potential impacts on equipment fidelity of time variations in process states under EMPC are not yet clear, though the example in Section 3.1 suggests that it is possible that there may be combinations of equipment designs and economically-optimal operating conditions determined by certain EMPC designs which could impact equipment fidelity. In the remainder of this section, we discuss some of the difficulties with developing appropriate process state constraints for EMPC, particularly within a framework based on traditional force, deformation, and fracture analyses, referring again to the chemical process example presented above at intervals to provide clarity to the discussion.

One of the challenges for developing EMPC's that utilize the state constraints of Eq. (6d) is ensuring that the constraints obtained within a traditional context based on forces, deformation, and fracture are comprehensive and sufficient for preventing material failure. Material mechanical behavior analysis is practiced with success in industry, and common techniques utilized in this direction would be expected to be useful for use in designing appropriate constraints for EMPC. In particular, it is reasonable to consider that the methodology of ensuring that the values of stresses experienced by a material, loads applied to a material, number of events experienced by a material, or time of use of a material remain far from the values of these quantities expected to cause failure in the material could be utilized in setting constraints. The ratio of the value which causes failure to the worst-case value experienced by the material during its use is known as a safety factor (Dowling, 2013), and an EMPC could be designed that requires that the worst-case stress, load, or event number in the equipment during operation must remain less than the failure value divided by a chosen safety factor (which then is a constraint on the stress, load, or number of events).

There is a good deal of freedom in selecting the criteria to be constrained by a safety factor, as well as in setting the value of the safety factor itself, that is typically handled practically using engineering judgment and experience. With regard to selecting the criteria to constrain, when static conditions are considered (i.e., failure mechanisms that depend on time are not considered), examples of constraints which might be considered are those based on stress or fracture. For stress-based criteria, the expected directions of the stresses that will be applied to the material must be evaluated. If the stresses are expected to be applied in a limited number of directions, and in particular in directions in which standard tests exist for evaluating material limitations (e.g., tension or torsion), it may be possible to apply constraints which require that the control actions computed by the EMPC result in material stresses being less than the value of the stresses associated with failure via these tests (with some conservatism applied in selecting the value of the stress associated with failure to account for the scatter in the materials testing data) via a safety factor. However, many materials are subject to complex loading during use, with the result that the stresses in the material are present in more directions than are typically considered during testing. The result is that, to determine which combination of stresses in multiple directions in the material correlates to a failure condition, failure criteria are often used which relate stresses in a material at a given location in that material to an effective stress value that can then be compared against a value from a material test (if the material is considered to be brittle, meaning that it does not sustain much deformation after yielding before fracture, the effective stress may be compared with the material's ultimate strength from a uniaxial tensile test, whereas if the material is ductile, meaning that it sustains more plastic deformation after yielding before fracture, the effective stress may be compared to the material's yield strength). In such cases, constraints may be considered using safety factors based on the effective stress values, perhaps throughout the material and over time to account for the fact that it would be undesirable for the failure criteria to be exceeded at any time during operation or at any position within the equipment.

As an example of constraints which might be developed for an EMPC, consider a brittle material under static loading for which the failure criterion selected for a multiaxial state of stress is a maximum normal stress fracture criterion (Dowling, 2013) in which the effective stress to be constrained at a given location in the material is the maximum principal normal stress (the maximum of the normal stresses obtained for a coordinate axis rotation giving no shear stress). In this case, it may be considered that when the effective stress is less than the ultimate strength of the material, the material does not fail. To account for the empiricism of this approach, safety factors can be applied to prevent failure even if this criterion is not the most accurate measure of failure in the material. If a safety factor of 3 is chosen, then the constraint which an EMPC might utilize could be as follows:

$$\sigma_e \leq \sigma_u/3 \tag{22}$$

where σ_e represents the value of the effective stress based on the maximum normal stress fracture criterion, and σ_u is the material's ultimate strength as determined via a uniaxial tension test. Other safety factor-based constraints could also be considered, with different formulations for the effective stress besides the maximum normal stress fracture criterion (e.g., Dowling (2013) suggests that the maximum normal stress fracture criterion may be reasonable for brittle materials when loaded primarily in tension, and that other criteria based on properties such as maximum shear stress in any direction at a given location in the material might be used for ductile materials), and then the value of the material property used in developing the constraint may be changed from σ_u to other material properties such as the stress at which the material yields, depending on the material properties and criterion being used. It should be noted that for EMPC design, especially in the case of time-varying loads or in cases where the geometry of the equipment results in areas of increased stress (stress raisers) compared to the rest of the part, it may be necessary to develop the constraints to hold at many locations throughout the material to ensure that they are not violated at critical locations over time since the equipment fidelity is safety-critical.

In addition to the types of constraints for static loading discussed in the prior paragraph (which assume that the material is free from defects such as cracks except that the values of material properties such as yield strength and ultimate strength used in the constraints implicitly account for unintended defects in test specimens that impact those experimental strength results), other analysis techniques can be utilized to protect against failure due to other mechanisms. For example, the techniques of fracture mechanics can be utilized to define safety factors related to (static) stresses which would cause a part to fracture if it has predefined cracks of certain sizes; with cracks of certain sizes, materials are more likely to fracture below the yield strength, particularly when the crack length is longer than a value called the transition crack length, which is dependent on the material and test and stress conditions (Dowling, 2013). One may also consider adding deformation-based constraints when an extent of deformation less than that expected at yield or fracture may result in failure in terms of an inability to use a component any longer. To be able to utilize constraints developed according to the above methods within an EMPC with the form of Eq. (6), it is necessary to relate the constraints involving safety factors to constraints on the process states. When this cannot be readily done, it may be desirable to consider modeling the equipment behavior in the EMPC as well and then constraining the equipment states explicitly.

The values of safety factors in equipment-based constraints must also be specified, and the value to utilize is a judgment call based on how well-understood the process/equipment and loads/stresses in service at hand are.

There are many factors in a stress/deformation/fracture framework that contribute to uncertainty that may need to be accounted for by using a more conservative safety factor, because this framework has aspects that are empirical and applied based on macroscopic phenomena, rather than the fundamental microscopic phenomena at play. An example of a factor which causes uncertainty is the empirical nature of methods for assessing conditions which cause failure, particularly in the case of multiaxial states of stress. For example, the yield strength itself is not an exact quantity. It is typically determined experimentally via uniaxial tensile tests where macroscopic test specimens are pulled at both ends until failure, and (macroscopic) stress and strain are measured in this test specimen within the ability of the equipment to capture these throughout the test. Microscopic variations between test specimens such as defects in the materials can cause different yield strengths to be obtained for the same material, and yield strength is somewhat difficult to define experimentally, as it is defined with respect to various different criteria that attempt to approximately locate where plastic deformation appears to begin to occur in the experimental results. Furthermore, though properties such as yield strength are typically determined via standardized tests such as uniaxial tensile tests, the stresses in a material are typically multiaxial. This fact can create very different failure conditions in a material than uniaxial stress conditions. For example, it is noted in Dowling (2013) that when a test specimen yields in a uniaxial tensile test with a yield strength σ_y in the y direction, then when transverse compressive stresses are added, the material may yield at a value of stress applied in the y direction that differs from σ_y. A traditional technique for accounting for the impacts of multiaxial stress conditions on component failure is to develop a function to relate stresses in a material to a single scalar that then would be compared to failure conditions to assess whether the material will fail as discussed above. There are different relationships which can be chosen between (e.g., the maximum shear stress criterion and octahedral shear stress yield criterion may be considered for ductile isotropic materials, with modifications to account for anisotropy, whereas the modified Mohr criterion may be utilized for brittle materials Dowling, 2013), which again adds uncertainty in the design of the EMPC constraints that may need to be accounted for with conservative constraints. A disadvantage of the macroscopic focus of some of the techniques in traditional stress and fracture-based analyses of material failure is that the results of tests that are used in assessing and constraining material fidelity depend on test conditions/test environment. An EMPC might modify the environment which the equipment experiences over time, meaning that techniques for relating phenomena which have not necessarily been tested to failure conditions must be used in defining the constraints. This indicates that the development of constraints for EMPC in a traditional fashion based on forces and deformations requires considerable experience in accounting for materials failure and requires a good degree of conservatism that may be undesirable to account for the number of uncertainties.

To demonstrate that conservatism may be undesirable, we can consider the implications of using large/conservative safety factors in the constraint design in more detail. For the example in Section 3.1, this would be analogous to restricting the upper bound on temperature more significantly to prevent the thermal stress in the pipe from exceeding a limit (this might be attempted if, for example, we did not want to check the exact spring constant of the bellows before designing the constraint, so instead we imposed a constraint in the EMPC requiring that the temperature remain less than the maximum value we had previously expected at steady-state, as that would then amount to an upper bound on temperature which the original equipment was known to be able to withstand). However, as discussed above, restricting the upper limit on temperature in this case restricts the profit that can be obtained under EMPC. Depending on the value of the spring constant, this could lead to an unnecessarily conservative constraint on temperature when considering the equipment design, as the equipment may be able to withstand higher temperatures. This indicates that for operating a process under EMPC, there is a potential that it may be more profitable to find a method for making the controller explicitly aware of the equipment behavior.

The above discussion suggests that a solution to the somewhat empirical nature of safety factor-based constraint development for an EMPC focused on preventing problematic conditions from being attained in equipment during operation may be to explore more fundamental molecular-level models of equipment behavior, rather than using models based on macroscopic behavior. This would be an interesting direction for future research, though it has the potential to require significant computation time, and this issue would need to be addressed. Potentially, techniques for either preventing or measuring the defects in materials could aid in reducing the need for conservative safety factors. However, there will still be a need for engineering judgment in determining what constitutes "failure," because failure of components is not defined via one characteristic at a microscopic or atomic level that can be fundamentally constrained. For example, failure is considered to occur in a component when due to issues such as deformation, a component no longer performs its intended function. This does not necessarily mean that fracture occurs or that a specific condition fundamental to the nature of materials has been reached; rather, it is application-specific. To see this, consider an example given in Dowling (2013), where "failure" for a building could mean that it sways in heavy winds in a manner that makes those in the building uncomfortable; essentially, some material condition must be associated to a qualitative notion of "discomfort" to set a limit on the material property that causes failure, and in another application, that same value of the material property may not be considered to be associated with failure. Some modes of failure would be expected to always need to be constrained against (e.g., equipment should not fracture), but other constraints on material behavior would fundamentally need to be application-specific, as definitions of "failure" are tied to the use of a component and therefore not only to its fundamental chemical nature.

An issue related to this is that because traditional deformation, stress, and fracture analyses do not provide a fundamental molecular-level perspective from which to analyze material behavior, they also do not provide a uniform framework for assessing all potential failure mechanisms which a material may face. This means that when developing an EMPC with constraints on failure mechanisms, engineers performing the EMPC design must think of every possible failure mechanism of the equipment under every possible operating condition for the process under EMPC (this may be particularly difficult to assess *a priori* in the case that there are disturbances) and then develop constraints that account for all of these. If a failure mechanism is overlooked, it is possible that the EMPC could lead to problems for the equipment, even if it contains constraints that prevent failure via other mechanisms which have not been overlooked. This can occur because not all failure types require the same conditions to occur, as the mechanisms which cause different failures are different. For example, if cyclical stresses are applied to a part over an extended time (e.g., for a certain number of cycles), the part may fail via a fatigue mechanism even if the stresses achieved were never greater than the yield stress. In that case, placing a constraint on the stress never exceeding the yield stress would not necessarily prevent the EMPC from computing input profiles that would cause the equipment to fail before it was expected.

Furthermore, because it can be difficult to predict the manner in which an EMPC may operate a process, it would not in general be expected that by fully analyzing all possible failure mechanisms at equilibrium conditions, one could come up with the right constraints for the EMPC. Specifically, non-equilibrium conditions also must be considered. Though one might consider including the partial differential equations which describe how stress, strain, and temperature vary in both space and time in the model used for making state predictions in EMPC, designing appropriate constraints on the variations of the equipment constraints over time is not straightforward because failure mechanisms for materials stemming from transients are fundamentally tied to microscopic-level phenomena. For example, one common technique for assessing how long it will take a material to fail under cyclically-varying loads is to perform high-cycle or low-cycle fatigue tests. In these tests, loads are varied according to a pre-determined cycle, and then the number of cycles until failure of the material is recorded. Though methods for relating even complex loading histories back to fatigue life test data obtained under different conditions can be used to develop safety factors for constraints, these methods would require conservatism for constraint design for EMPC. A molecular-level model of the mechanism which leads to failure due to fatigue may be beneficial in this case, and the states of such a model could be constrained.

Time is well-known to impact various phenomena related to material failure; for example, when cracks are present in a material, the manner in which loading is applied over time or the manner in which environmental effects impact a material over time can play a significant role in setting the stress which causes fracture (Dowling, 2013). Furthermore, temperature may vary over time for a process under EMPC, and cracked materials are known to fail via fracture at different stresses for different temperatures. This suggests that time variations in temperature would be expected to cause some time variation in the upper limits which should be imposed on material conditions like stress and strain in EMPC design unless a conservative upper bound is utilized that takes into account the worst-case temperature expected under EMPC (in the case that LEMPC is used, this could be readily determined *a priori* by looking at temperatures on the boundary of the stability region). With a less conservative approach, the upper bound on stress would need to be written as an explicit function of temperature, which is varying over time in accordance with the control actions being computed by the EMPC.

It is important to consider how constraints may impact the optimal solution when attempting to use cycles-until-failure data in setting constraints within an EMPC, even when it produces almost cyclic behavior of a process state such as temperature that may result in some cyclic variations in equipment states such as the temperature in the material. For example, consider again the example of Section 3.1 and consider that the constraint on the feedstock from the EMPC of Fig. 6 continues to be enforced over every hour, but that the process is operated for 5 h. In that case, concentration and temperature profiles are set up as shown in Fig. 9 which appear almost cyclic due to the fact that the constraint of Eq. (14) is enforced by requiring the time-averaged value of u_1 to be equal to its steady-state value at the end of every hour, leading to a constraint enforced in a periodic fashion and hence to the periodicity in the trajectories. When considering a constraint to impose in the EMPC, it may at first seem intuitive to seek to determine, perhaps via a thermal cycling test, what number of cycles of temperature leads to failure of the process equipment due to thermal fatigue, and then to place a constraint in the EMPC requiring that the number of cycles of temperature must be less than that number within a given timeframe corresponding to the expected use life of the material. Neglecting for a moment any considerations with respect to how to enforce such a material life-based constraint over a finite prediction horizon, we can see upon further probing of this constraint that it is poorly defined. For example, consideration must be given to what defines a temperature cycle. While one could seek to impose a constraint requiring that, for example, the temperature not reach the maximum value of the temperature in Fig. 9 followed by the minimum value of temperature in Fig. 9 more than the allowable number of times within the prediction horizon, this constraint would not guarantee that some other time-varying operating policy, or even another cycle with some other period or amplitude of variation, was set up. Safety factors can be developed related to fatigue life test data at other conditions that could be used in defining constraints in the EMPC; methods have also been explored for relating irregular loading to fatigue life test data which could be considered for constraint development (Dowling, 2013). However, a desirable constraint could be one which fundamentally constrains the material damage, rather than empiricisms related to the cycle itself. In this analysis, we see that placing constraints solely on process state variables, rather than equipment states, may prove insufficient for constraining the material behavior within an EMPC when damage related to time-varying effects is considered. Furthermore, because the cycling frequency in Fig. 9 is induced via the manner in which the constraint of Eq. (14) is enforced, this indicates that the manner in which the controller is designed should take into account the equipment considerations (e.g., perhaps the constraint should be enforced differently to avoid the manner of cycling in Fig. 9).

Remark 3. The discussion in this section helps to clarify the question which is being asked in this work, which is: how do we begin to thoroughly analyze the implications of EMPC for process equipment before utilizing it to ensure that process safety is maintained after EMPC is deployed? This question is not addressed explicitly via materials modeling in industrial implementations of MPC, and it is therefore necessary to clarify why it is being asked for industrial implementations of EMPC. One of the challenges with EMPC that is not faced by traditional tracking MPC is that the loading to be experienced by the equipment is not necessarily obvious *a priori*, as the EMPC is not necessarily designed to force the process to operate at a steady-state like a tracking MPC is. In the steady-state case, the expected loading can be more readily analyzed *a priori* and the equipment design can be modified such that it is able to withstand the expected operating conditions, with required safety factors on every mode of failure considered at the equipment

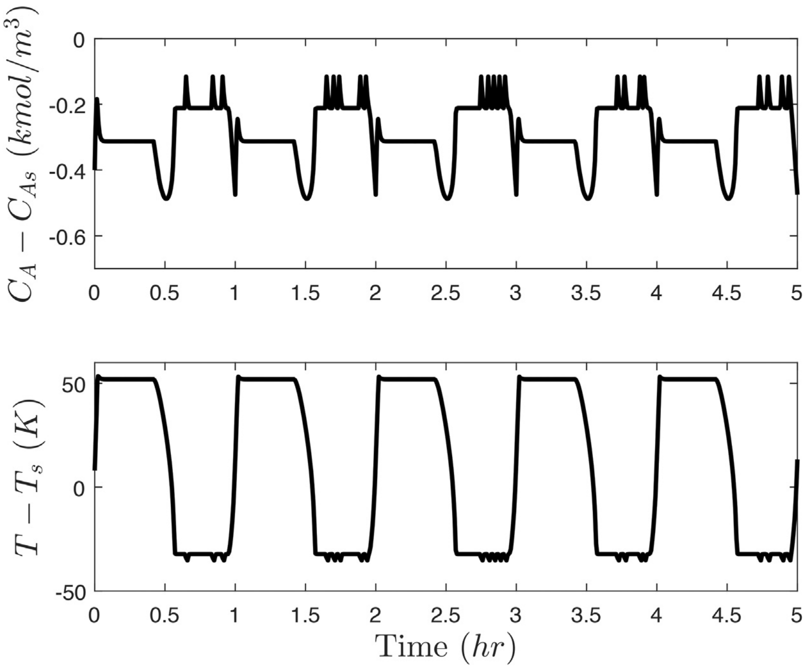

Fig. 9 – States over five hours of operation for the process of Eqs. (8)–(9) under EMPC with the slack variables in the constraints of Eqs. (15)–(16).

design stage. It therefore is not necessary to account for the equipment limitations in the control design, as the equipment has been designed to withstand the steady-state conditions. However, in the case of EMPC, it becomes necessary to consider new operating conditions which vary dynamically over time and therefore are not necessarily straightforward to fully assess *a priori* so that the equipment can be designed to handle all of it. Furthermore, it would be expected that some implementations of EMPC may be applied using equipment that was previously designed for use under steady-state operation and now is being used under EMPC; when this occurs, it is not possible to impact the mechanical design of the equipment to account for the new operating conditions, so the controller itself may need to account for the equipment. Furthermore, conservative safety factors are not detrimental to the value of the objective function (which can be considered to be the desired profit metric) when it is desirable to operate the process at a steady-state, because then the conservatism in the safety factors which restricts the process states to remain closer to the steady-state via state constraints does not force the state away from the optimal value it would take according to the objective function as it may in the case of EMPC.

Remark 4. It should be clarified that in this work, we are seeking to understand the conditions under which time-varying operation could lead to failure, and then how state constraints might be designed to prevent the controller from calculating a time-varying operating policy that would lead to failure. Though there are some engineering applications where the goal is to create failure of a material (e.g., causing fracture of rock formations to facilitate hydraulic fracturing (Siddhamshetty et al., 2018b), where models of fracturing (Kim and Moridis, 2013) have been developed and used in control design with the goal of facilitating fracturing via the controller (Siddhamshetty et al., 2018a)), our intent in this work is not to cause failure with the controller (in the case of failure, significant safety concerns could arise that could lead to process shut-down and equipment replacement), but rather to better understand how EMPC might impact processes on a practical level that accounts for how the operating conditions set up by the controller could impact equipment.

5. New considerations in accounting for equipment-control interactions in EMPC

In this section, we review some conclusions from the simulations in Section 3.1 that reveal new considerations that will need to be handled when considering equipment-control interactions in EMPC, both for cases where the process states are constrained and cases where models for equipment behavior are directly constrained. The example of Section 3.1, though for a heavily simplified situation and with a spring constant that is likely much stiffer than those which would typically be installed, nevertheless indicates a number of significant conclusions about potential practical implications of the use of EMPC and EMPC accounting for equipment-control interactions for a chemical process.

The first conclusion is that the details of equipment design (in this example, factors such as the pipe length, whether there is a bellows joint and what its spring constant is, and whether the pipe is rigidly fixed on any side) for units in a process under EMPC may play a significant role in the analysis of whether the use of EMPC for such a process in place of a controller that enforces steady-state operation may be considered without some level of control/equipment co-design, such as incorporating the equipment limitations in the EMPC by modifying the constraints. The example indicates that though typical values of k_s for a bellows joint would cause the piping to have no issues with the added thermal stress due to the EMPC-induced temperature change in the pipe compared to the expected thermal stress at steady-state conditions, a specialty equipment design could be negatively impacted by the added stress. The significance of this is that it will not be possible to make any general conclusions about whether EMPC that does not explicitly account for material behavior will or will not cause negative effects for process equipment - this will need to be evaluated by each potential EMPC user for all of their equipment before employing EMPC. It is noted that the answer will depend both on the equipment construction as well as the EMPC design. For example, if the profit metric to be used in the example in Section 3.1 had been a metric that forced the closed-loop state to remain at the operating steady-state, then the EMPC-equipment combination would not be expected to cause issues for the equipment fidelity. Similarly, when k_s is low but the EMPC is that used in Fig. 1, it is not expected that the EMPC-equipment combination causes issues for the equipment. However, Section 3.1 also presents combinations of EMPC designs with equipment that have the potential to be problematic.

A second conclusion is that the results above showcase that the decisions made by an EMPC controlling an upstream process (in the case that a centralized EMPC is not used to control an entire plant) will impact downstream processes, and this may result in constraints in EMPC intended to account for how the upstream process impacts the downstream process. No aspect of the process can be neglected when exploring what the effects of the use of EMPC for maximizing the profit for the process will be, including units such as pipes which might otherwise be considered to be able to be neglected for the purposes of control design or at most represented with a time delay in a dynamic model. This is further demonstrated by seeking to analyze how equipment behavior might be modeled more rigorously from a solid mechanics perspective. For example, consider the following system of partial differential equations, which describe the relationships between various stresses at a point in a material at mechanical equilibrium with no body forces such as gravity or stresses related to thermal effects (Shames, 1989):

$$\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} = 0 \tag{23}$$

$$\frac{\partial \tau_{yx}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{yz}}{\partial z} = 0 \tag{24}$$

$$\frac{\partial \tau_{zx}}{\partial x} + \frac{\partial \tau_{zy}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} = 0 \tag{25}$$

where τ_{xx}, τ_{yy} and τ_{zz} are normal stresses in the x, y, and z directions on an infinitesimal volume of material, and $\tau_{xy} = \tau_{yx}$, $\tau_{xz} = \tau_{zx}$ and $\tau_{yz} = \tau_{zy}$ are shear stresses on the various faces of the material. The boundary conditions for Eqs. (23)-(25) will play a significant role in setting the stress distribution, and they may depend on the adjacent equipment. This may also be indicated for the case in which it is desired to analyze the temperature in the pipe in Section 3.1 in three dimensions, where the pipe temperature boundary conditions at the two ends of the pipe will need to be specified and will depend on the temperature of adjacent equipment or heat fluxes from/to this equipment. This analysis again indicates that a plant-wide modeling effort would be required to fully develop appropriate models and boundary conditions for investigating whether EMPC would be suitable for a process, or if it might cause material damage that must be constrained before it would be suitable. However, utilizing engineers at a company to develop such models would not be possible, and solving such large-scale models within an EMPC would be computationally time-consuming and potentially intractable. This is particularly the case since the required models may be systems of partial differential equations. Furthermore, because we see above that detailed equipment design and material properties play a role in the development of appropriate constraints for an EMPC that account for equipment-control interactions, it would be necessary to consider modifications to the EMPC after routine work such as maintenance is performed to ensure that the EMPC still appropriately constrains the equipment states after modifications. If EMPC accounting for equipment-control interactions is to be considered, techniques must be explored for reducing or eliminating engineering effort in the development of process-equipment models and for automatically updating the models when modifications to the process or equipment are made.

One potential new method for reducing the need to impose constraints in EMPC (with the goal of reducing computational effort required for EMPC) would be to select equipment materials and designs in light of control. For example, in the case above in which the temperature is restricted to prevent thermal stress, the profit is less than it would be if the closed-loop state was free to take any value within the stability region Ω_ρ when $\rho = 300$ (i.e., where in this Ω_ρ, the upper limit on the temperature is higher than 450 K). For example, to be able to utilize this Ω_ρ that gives greater profitability but without exceeding the design stress, a less stiff bellows joint could be utilized as discussed above. If the bellows joint is sufficiently flexible such that all problematic temperatures are outside of the stability region, no additional modeling of process equipment or constraints on the equipment needs to be included in EMPC (however, this holds only if we are looking at this single failure scenario and if no maintenance is performed that modifies the equipment design by, for example, replacing the bellows joint).

6. Conclusions

This work developed a preliminary investigation into how to evaluate whether EMPC designs could pose issues for process equipment material fidelity. It investigated the extent to which process state constraints are sufficient for ensuring that an EMPC will not compromise process equipment material fidelity. The extent to which the traditional methods of modeling equipment behavior for mechanical design, as well as the traditional methods for accounting for equipment-control interactions in EMPC via process state constraints, are able to handle the implications of time-varying operation for process equipment was explored. The work overall indicated that despite some of the benefits of stress, deformation, and fracture-based techniques for modeling equipment behavior, it is likely that the use of these macroscopic modeling techniques would require some conservatism in developing constraints that has the potential to reduce profits under EMPC. A chemical process example aided in illustrating a number of points regarding the proposed technique.

Future work will seek to further investigate materials modeling in control with the goal that models, allowing predictions for how the material would behave in the future, could be used in selecting control actions or alerting engineers in the event that predictions appear to involve failure. We also plan to consider incorporating partial differential equation models related to equipment states such as temperature and stress/deformation in multiple dimensions in EMPC design to investigate the effect on the control actions if equipment states are directly constrained, and to address challenges expected in this direction such as the development of appropriate constraints and exploring computation time reduction techniques.

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