

Predictive control of transport-reaction processes

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Abstract

This work focuses on the development of computationally efficient predictive control algorithms for nonlinear parabolic and hyperbolic PDEs with state and control constraints arising in the context of transport-reaction processes. We first consider a diffusion-reaction process described by a nonlinear parabolic PDE and address the problem of stabilization of an unstable steady-state subject to input and state constraints. Galerkin's method is used to derive finite-dimensional systems that capture the dominant dynamics of the parabolic PDE, which are subsequently used for controller design. Various model predictive control (MPC) formulations are constructed on the basis of the finite dimensional approximations and are demonstrated, through simulation, to achieve the control objectives. We then consider a convection-reaction process example described by a set of hyperbolic PDEs and address the problem of stabilization of the desired steady-state subject to input and state constraints, in the presence of disturbances. An easily implementable predictive controller based on a finite dimensional approximation of the PDE obtained by the finite difference method is derived and demonstrated, via simulation, to achieve the control objective. © 2005 Elsevier Ltd. All rights reserved.

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1. Introduction

Transport-reaction processes are characterized by significant spatial variations and nonlinearities due to the underlying diffusion and convection phenomena and complex reaction mechanisms, respectively. The dynamic models of transport-reaction processes over finite spatial domains in which both the diffusion and convection transport mechanisms are important typically consist of parabolic partial differential equation (PDE) systems whose spatial differential operators are characterized by a spectrum that can be partitioned into a finite (possibly unstable) slow part and an infinite stable fast complement (Curtain & Pritchard, 1978). The traditional approach to control of linear/quasi-linear parabolic PDEs involves the application of spatial discretization techniques to the PDE system to derive systems of ordinary differential equations (ODEs) that accurately describe the dynamics of the dominant (slow) modes of the PDE system. These

finite-dimensional systems are subsequently used as the basis for the synthesis of finite-dimensional controllers (e.g., see Balas, 1979; Curtain, 1982; Ray, 1981). A potential drawback of this approach, especially for quasi-linear parabolic PDEs, is that the number of modes that should be retained to derive an ODE system that yields the desired degree of approximation may be very large, leading to complex controller design and high dimensionality of the resulting controllers.

Motivated by these considerations, significant recent work has focused on the development of a general framework for the synthesis of low-order controllers for quasi-linear parabolic PDE systems – and other highly dissipative PDE systems that arise in the modeling of spatially-distributed systems including fluid dynamic systems – on the basis of low-order nonlinear ODE models derived through a combination of Galerkin's method (using analytical or empirical basis functions) with the concept of inertial manifolds (Christofides, 2001). Using these order reduction techniques, a number of control-relevant problems, such as nonlinear and robust controller design, dynamic optimization, and

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control under actuator saturation have been addressed for various classes of dissipative PDE systems (e.g., see Armaou & Christofides, 2002a, 2002b; Baker & Christofides, 2000; Christofides & Daoutidis, 1997; El-Farra, Armaou, & Christofides, 2003 and the book Christofides, 2001 for results and references in this area).

When convective mechanisms dominate over diffusive ones, transport-reaction processes can be adequately described by systems of hyperbolic PDEs, whose spatial differential operator possesses different features than the one associated with parabolic PDEs. Specifically, all the eigenmodes of the spatial differential operator of hyperbolic PDEs contain the same, or nearly the same amount of energy, and thus, high order finite dimensional approximation is necessary to accurately describe the dynamic behavior of hyperbolic PDEs. This feature unfortunately prevents the application of aforementioned reduction techniques, to derive reduced-order models that approximately describe the dynamics of the PDE system, and motivates addressing the control problem on the basis of the infinite-dimensional model itself. Following this approach, a methodology based on combination of the method of characteristics and sliding mode techniques was proposed for the design of distributed state feedback controllers (Hanczyc & Palazoglu, 1995; Sira-Ramirez, 1989). Also, geometric control and Lyapunov-based control methodologies were developed for the design of nonlinear (Christofides & Daoutidis, 1996) and robust (Christofides & Daoutidis, 1998) controllers. Within the framework of model predictive control, in (Shang, Forbes, & Guay, 2004), a model predictive control (MPC) formulation was developed on the basis of an ODE model derived by the method of characteristics.

The control methods proposed in the above works, for both nonlinear parabolic and hyperbolic PDEs, however, do not address the issue of state constraints in the controller design. Operation of transport-reaction processes typically requires that the state of the closed-loop system be maintained within certain bounds to achieve acceptable performance (for example, requiring reactor temperature not to exceed a certain value or requiring a product concentration not to drop below some purity requirement). Handling both state and control constraints – the latter typically arising due to the finite capacity of control actuators – in the design of the feedback controller, therefore, is an important consideration.

Model predictive control, also known as receding horizon control, is a popular control method for handling constraints (both on manipulated inputs and state variables) within an optimal control setting. In MPC, the control action is obtained by solving repeatedly, on-line, a finite-horizon constrained open-loop optimal control problem. The popularity of this approach stems largely from its ability to handle, among other issues, multi-variable interactions, constraints on controls and states, and optimization requirements. Numerous research studies have investigated the properties of model predictive controllers and led to a plethora of MPC formulations that focus on a number of control-relevant

issues, including issues of closed-loop stability, performance, implementation and constraint satisfaction (e.g., see Allgower & Chen, 1998; Garcia, Prett, & Morari, 1989; Mayne, Rawlings, Rao, & Scokaert, 2000; Rawlings, 2000 for surveys of results and references in this area).

Most of the research in the area of predictive control, however, has focused on lumped-parameter processes modeled by ODE systems. Compared with lumped-parameter systems, the problem of designing predictive controllers for distributed parameter systems, modeled by PDEs, has received much less attention. Of the few results available on this problem, some have focused on analyzing the receding horizon control problem on the basis of the infinite-dimensional system using control Lyapunov functionals (e.g., Ito & Kunisch, 2002), while others have used spatial discretization techniques such as finite differences (e.g., Dufour, Touré, Blanc, & Laurent, 2003) to derive approximate ODE models (of possibly high-order) for use within the MPC design, thus leading to computationally expensive model predictive control designs that are, in general, difficult to implement on-line. In a previous work (Dubljevic, El-Farra, Mhaskar, & Christofides, submitted for publication), we considered linear parabolic PDE systems and derived finite-dimensional predictive controller formulations that handled the objectives of state and input constraints satisfaction and stabilization of the infinite dimensional system.

In this work, we focus on the development of computationally efficient predictive control algorithms for nonlinear parabolic and hyperbolic PDEs with state and control constraints arising in the context of transport-reaction processes. The rest of the paper is organized as follows: in Section 2, we consider a diffusion-reaction process described by a nonlinear parabolic PDE and address the problem of stabilization of an unstable steady-state subject to input and state constraints. Galerkin's method is used to derive finite-dimensional systems that capture the dominant dynamics of the parabolic PDE, which are subsequently used for controller design. Various MPC formulations are constructed on the basis of the finite dimensional approximations and are demonstrated, through simulation, to achieve the control objectives. Next, in Section 3, we consider a convection-reaction process example described by a set of hyperbolic PDEs and address the problem of stabilization of the desired steady-state subject to input and state constraints, in the presence of disturbances. An easily implementable predictive controller based on a finite dimensional approximation of the PDE obtained by the finite difference method is derived and demonstrated, via simulation, to achieve the control objective.

2. Predictive control of diffusion-reaction processes

2.1. Motivating example

In this section, we consider a representative example of a diffusion-reaction system described by a parabolic PDE of

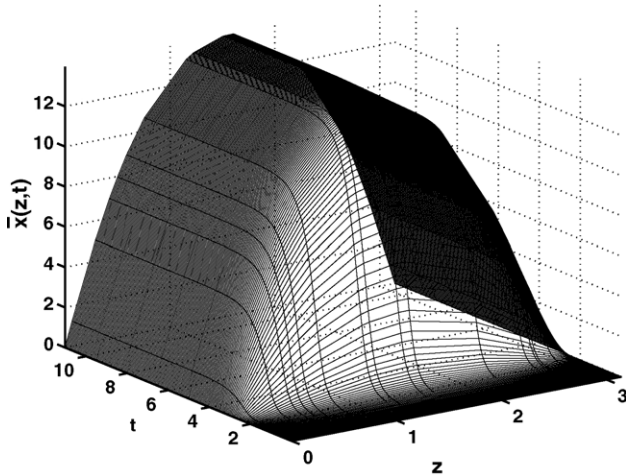


Fig. 1. Open-loop profile showing the instability of the $\bar{x}(z, t) = 0$ steady-state.

the following form:

$$\frac{\partial \bar{x}}{\partial t} = \frac{\partial^2 \bar{x}}{\partial z^2} + \beta_T (e^{-\gamma/(1+\bar{x})} - e^{-\gamma}) - \beta_U \bar{x} + \beta_U \sum_{i=1}^m b_i(z) u_i(t)$$

$$\bar{x}(0, t) = 0, \quad \bar{x}(\pi, t) = 0, \quad \bar{x}(z, 0) = x_0(z)$$

(1)

where \bar{x} denotes the dimensionless state of the system, β_T denotes a dimensionless heat of reaction, γ denotes a dimensionless activation energy, β_U denotes a dimensionless heat transfer coefficient, $u_i(t)$ denotes the manipulated input and $b_i(z)$ is the actuator distribution function of the i th actuator, chosen to be $b_i(z) = 1/\mu$ for $z \in [z_{ai} - \mu, z_{ai} + \mu]$ and $b_i(z) = 0$ elsewhere in $[0, \pi]$, where μ is a small positive real number and z_{ai} is the center of the interval where actuation is applied. The following typical values are given to the process parameters: $\beta_T = 50$, $\beta_U = 2$ and $\gamma = 4$. For these values, it was verified that the operating steady-state, $\bar{x}(z, t) = 0$, is an unstable one, as can be seen from Fig. 1. The control objective is to stabilize the state profile at the unstable zero steady-state subject to the following input and state constraints

$$u_i^{\min} \leq u_i \leq u_i^{\max} \tag{2}$$

$$\chi^{\min} \leq \int_0^\pi r(z) \bar{x}(z, t) dz \leq \chi^{\max} \tag{3}$$

where $u_i^{\min} = -10$, $u_i^{\max} = 10$, for $i = 1, 2$, $\chi^{\min} = -0.035$, $\chi^{\max} = 2$. The state constraints distribution function, $r(\cdot)$, is chosen to be $r(z) = \delta(z - z_c)$ for $z \in [0, \pi]$ and $z_c = 1.156$. This choice of $r(z)$ implies that the state constraints are to be enforced only at a single point in the spatial domain, i.e., $-0.035 \leq \bar{x}(z_c, t) \leq 2$. For this system, we consider the first two eigenvalues as the dominant ones and use two point control actuators ($m = 2$), with finite support, centered at $z_{a1} = \pi/3$ and $z_{a2} = 2\pi/3$, to achieve the control objective subject to the constraints of Eqs. (2) and (3).

2.2. Galerkin's method

To present our results, we first formulate the PDE of Eq. (1) as an infinite dimensional system in the Hilbert space $\mathcal{H}([0, \pi]; \mathbb{R})$, with \mathcal{H} being the space of measurable functions defined on $[0, \pi]$, with inner product and norm:

$$(\omega_1, \omega_2) = \int_0^\pi (\omega_1(z), \omega_2(z))_{\mathbb{R}} dz,$$

$$\|\omega_1\|_2 = (\omega_1, \omega_1)^{1/2} \tag{4}$$

where ω_1, ω_2 are two elements of $\mathcal{H}([0, \pi]; \mathbb{R})$ and the notation $(\cdot, \cdot)_{\mathbb{R}}$ denotes the standard inner product in \mathbb{R} . Defining the state function x on $\mathcal{H}([0, \pi]; \mathbb{R})$ as:

$$x(t) = \bar{x}(z, t), \quad t > 0, \quad z \in [0, \pi], \tag{5}$$

the operator \mathcal{A} in $\mathcal{H}([0, \pi]; \mathbb{R})$ as:

$$\mathcal{A}x = \frac{\partial^2 \bar{x}}{\partial z^2}, \quad x \in D(\mathcal{A}) = \left\{ x \in L_2([0, \pi]; \mathbb{R}) : \frac{dx}{dz}, \right.$$

$$\left. x, \text{ abs. cont.}, \frac{d^2x}{dz^2} \in L_2([0, \pi]; \mathbb{R}), x(0) = 0, x(\pi) = 0 \right\} \tag{6}$$

and the input operators as:

$$\mathcal{B}u = \sum_{i=1}^m b_i u_i, \tag{7}$$

the system of Eq. (1) takes the form:

$$\dot{x} = \mathcal{A}x + \mathcal{F}(x) + \mathcal{B}u, \quad x(0) = x_0 \tag{8}$$

where $x_0 = x_0(z)$. For the operator \mathcal{A} , the eigenvalue problem takes the form

$$\frac{d^2 \phi_j}{dz^2} = \lambda_j \phi_j \tag{9}$$

subject to

$$\phi_j(0) = \phi_j(\pi) = 0 \tag{10}$$

The above eigenvalue problem can be solved analytically and its solution yields

$$\lambda_j = -j^2, \quad \phi_j(z) = \sqrt{\frac{2}{\pi}} \sin(jz), \quad j = 1, \dots, \infty \tag{11}$$

Throughout the rest of the paper, the notation $|\cdot|$ will be used to denote the standard Euclidian norm in \mathbb{R}^n , while the notation $|\cdot|_Q$ will be used to denote the weighted norm defined by $|x|_Q^2 = x' Q x$, where Q is a positive-definite matrix and x' denotes the transpose of x . Finally the notation $\|\cdot\|_2$ will be used to denote the L_2 norm (as defined in Eq. (4) above) associated with a finite or infinite dimensional Hilbert space.

Next, we apply standard Galerkin's method to the infinite-dimensional system of Eq. (8) to derive a finite-dimensional system. Let $\mathcal{H}_s, \mathcal{H}_f$ be modal subspaces of \mathcal{A} , defined as $\mathcal{H}_s =$

$\text{span}\{\phi_1, \phi_2, \dots, \phi_m\}$ and $\mathcal{H}_f = \text{span}\{\phi_{m+1}, \phi_{m+2}, \dots\}$ (the existence of $\mathcal{H}_s, \mathcal{H}_f$ follows from the properties of \mathcal{A}). Defining the orthogonal projection operators, P_s and P_f , such that $x_s = P_s x, x_f = P_f x$, the state x of the system of Eq. (8) can be decomposed as:

$$x = x_s + x_f = P_s x + P_f x \quad (12)$$

Applying P_s and P_f to the system of Eq. (8) and using the above decomposition for x , the system of Eq. (8) can be rewritten in the following equivalent form

$$\begin{aligned} \frac{dx_s}{dt} &= \mathcal{A}_s x_s + \mathcal{F}_s(x_s, x_f) + \mathcal{B}_s u, \\ \frac{dx_f}{dt} &= \mathcal{A}_f x_f + \mathcal{F}_f(x_s, x_f) + \mathcal{B}_f u \\ x_s(0) &= P_s x(0) = P_s x_0 \\ x_f(0) &= P_f x(0) = P_f x_0 \end{aligned} \quad (13)$$

where $\mathcal{A}_s = P_s \mathcal{A}, \mathcal{B}_s = P_s \mathcal{B}, \mathcal{A}_f = P_f \mathcal{A}, \mathcal{B}_f = P_f \mathcal{B}$. In the above system, \mathcal{A}_s is a diagonal matrix of dimension $m \times m$ of the form $\mathcal{A}_s = \text{diag}\{\lambda_j\}$ (λ_j are possibly unstable eigenvalues of \mathcal{A}_s) and \mathcal{A}_f is an unbounded differential operator which is exponentially stable (following from the fact that $\lambda_{m+1} < 0$ and the selection of $\mathcal{H}_s, \mathcal{H}_f$). In the remainder of the paper, we will refer to the x_s - and x_f -subsystems in Eq. (13) as the slow and fast subsystems, respectively.

2.3. Control problem formulation

Referring to the system of Eq. (8), we consider the problem of asymptotic stabilization of the origin, subject to the following control and state constraints:

$$\dot{x}(t) = \mathcal{A}x(t) + \mathcal{F}(x(t)) + \mathcal{B}u(t), \quad x(0) = x_0 \quad (14)$$

$$u_i^{\min} \leq u_i(t) \leq u_i^{\max} \quad (15)$$

$$\chi^{\min} \leq (r, x(t)) \leq \chi^{\max} \quad (16)$$

This problem will be addressed within an MPC framework where the control, at state x and time t , is conventionally obtained by solving, on-line, a finite-horizon constrained optimal control problem of the form

$$P(x, t) : \min\{J(x, t, u(\cdot)) | u(\cdot) \in S\} \quad (17)$$

$$\begin{aligned} \text{s.t. } \dot{x}(\tau) &= \mathcal{A}x(\tau) + \mathcal{F}(x(\tau)) + \mathcal{B}u(\tau) \\ \chi^{\min} &\leq (r, x(\tau)) \leq \chi^{\max}, \quad \tau \in [t, t + T] \end{aligned} \quad (18)$$

where $S = S(t, T)$ is the family of piecewise continuous functions (functions continuous from the right), with period Δ , mapping $[t, t + T]$ into $\mathcal{U} := \{u \in \mathbb{R}^m : u_i^{\min} \leq u_i \leq u_i^{\max}, i = 1, \dots, m\}$, and T is the specified horizon. A control $u(\cdot)$ in S is characterized by the sequence $u[k]$, where $u[k] := u(k\Delta)$, and satisfies $u(t) = u[k]$ for all $t \in [k\Delta, (k + 1)\Delta)$. The performance index is given by

$$\int_t^{t+T} [q \|x^u(\tau; x, t)\|_2^2 + |u(\tau)|_R^2] d\tau + F(x(t + T)) \quad (19)$$

where $q > 0, R$ is a strictly positive definite matrix, $x^u(\tau) = x(\tau; x, t)$ denotes the solution of Eq. (8), due to control u , with initial state x at time t , and $F(\cdot)$ denotes the terminal penalty. The minimizing control $u^0(\cdot) \in S$ is then applied to the system over the interval $[k\Delta, (k + 1)\Delta]$ and the procedure is repeated indefinitely. This defines an implicit model predictive control law

$$M(x) := u^0(t; x, t) \quad (20)$$

Remark 1. It is well known that the control law defined by Eqs. (17)–(20) is not necessarily stabilizing (even for the finite-dimensional system). For finite-dimensional systems, the issue of closed-loop stability is usually addressed by means of imposing suitable penalties and constraints on the state at the end of the optimization horizon (e.g., see Allgower & Chen, 1998; Bemporad & Morari, 1999; Mayne et al., 2000 for surveys of different approaches). Furthermore, for a given stabilizing MPC formulation, it is in general difficult to compute the set of initial conditions starting from where the closed-loop system is guaranteed to be stable. In one approach, the implementation of MPC is complemented with Lyapunov-based bounded control in a way that allows both approaches to complement the stability and performance properties of each other, and has been utilized for state (El-Farra, Mhaskar, & Christofides, 2004b) and output (Mhaskar, El-Farra, & Christofides, 2004) feedback stabilization of linear systems, nonlinear systems (El-Farra, Mhaskar, & Christofides, 2004a) and nonlinear systems with uncertainty (Mhaskar, El-Farra, & Christofides, 2005), subject to input constraints. For the simulation example presented here, and for the choice of MPC parameters and initial conditions, the closed-loop system under MPC was found to be stabilizing; we therefore do not impose stability constraints in the optimization problem, but focus on the task of state constraint satisfaction.

One possible way to formulate the constrained nonlinear MPC problem is to design it on the basis of the full system of Eq. (13). The control action is then obtained by solving the following optimization problem:

$$\min_u \int_t^{t+T} [q_s \|x_s(\tau)\|_2^2 + q_f \|x_f(\tau)\|_2^2 + |u(\tau)|_R^2] d\tau \quad (21)$$

$$\begin{aligned} \text{s.t. } \dot{x}_s(\tau) &= \mathcal{A}_s x_s(\tau) + \mathcal{F}_s(x_s(\tau), x_f(\tau)) + \mathcal{B}_s u(\tau) \\ \dot{x}_f(\tau) &= \mathcal{A}_f x_f(\tau) + \mathcal{F}_f(x_s(\tau), x_f(\tau)) + \mathcal{B}_f u(\tau) \\ u(\tau) &\in \mathcal{U} \\ \chi^{\min} &\leq (r, x(\tau)) \leq \chi^{\max}, \quad \tau \in [t, t + T] \end{aligned} \quad (22)$$

where q_s, q_f are positive real numbers and R is a positive definite matrix. The above formulation includes penalties on both the slow and fast states and uses models that describe their evolution for prediction purposes. The infinite dimensional nature of the controller, however, renders it unsuitable for the purpose of online implementation. We now present and compare nonlinear MPC formulations that differ in the

way the state constraints are enforced and in the construction of the performance functional in the optimization problem.

2.4. Low-order predictive control formulation

In this formulation, the predictive controller is designed on the basis of the low-order, finite-dimensional slow subsystem describing the evolution of the x_s states (the fast subsystem is neglected). Specifically, the nonlinear MPC law is obtained by solving, in a receding horizon fashion, the following optimization problem:

$$\min_u \int_t^{t+T} [q_s \|x_s(\tau)\|_2^2 + |u(\tau)|_R^2] d\tau \quad (23)$$

$$\begin{aligned} \text{s.t. } \dot{x}_s(\tau) &= \mathcal{A}_s x_s(\tau) + \mathcal{F}_s(x_s(\tau), 0) + \mathcal{B}_s u(\tau) \\ u(\tau) &\in \mathcal{U} \\ \chi^{\min} &\leq (r, x_s(\tau)) \leq \chi^{\max}, \quad \tau \in [t, t + T] \end{aligned} \quad (24)$$

To simplify the presentation of the results, we will work with the amplitudes of the eigenmodes of the PDE of Eq. (1). Specifically, using Galerkin’s method, we derive the following high-order ODE system that describes the temporal evolution of the amplitudes of the first l eigenmodes:

$$\begin{aligned} \dot{a}_s(t) &= A_s a_s(t) + F_s(a_s(t), a_f(t)) + B_s u(t) \\ \dot{a}_f(t) &= A_f a_f(t) + F_f(a_s(t), a_f(t)) + B_f u(t) \end{aligned} \quad (25)$$

where $a_s(t) = [a_1(t) a_2(t)]'$, $a_f(t) = [a_3(t) a_4(t) \cdots a_l(t)]'$, $a_i(t) \in \mathbb{R}$ is the modal amplitude of the i th eigenmode, the notation a_s denotes the transpose of a_s , $u(t) = [u_1(t) u_2(t)]'$, the matrices A_s and A_f are diagonal matrices, given by $A_s = \text{diag}\{\lambda_i\}$, for $i = 1, 2$ and $A_f = \text{diag}\{\lambda_i\}$, for $i = 3, \dots, l$. B_s and B_f are a 2×2 and $(l - 2) \times m$ matrices, respectively whose (i, j) th element is given by $B_{ij} = (b_j(z), \phi_i(z))$. Note that $\bar{x}(z, t) = \sum_{i=1}^l a_i(t) \phi_i(z)$, $x_s(t) = a_1(t) \phi_1 + a_2(t) \phi_2$, $x_f(t) = \sum_{i=3}^l a_i(t) \phi_i$ and that $(x_s(t), \phi_i) = a_i(\phi_i, \phi_i)$. Using these projections, the state constraints of Eq. (3) can be expressed as constraints on the modal amplitudes as follows:

$$\chi^{\min} \leq \sum_{i=1}^2 a_i(t) \phi_i(z_c) + \sum_{i=3}^l a_i(t) \phi_i(z_c) \leq \chi^{\max} \quad (26)$$

The MPC formulation of Eq. (24), when written in terms of the amplitudes of the eigenmodes takes the following form:

$$\min_u \int_t^{t+T} [q_s |a_s(\tau)|^2 + |u(\tau)|_R^2] d\tau \quad (27)$$

$$\begin{aligned} \text{s.t. } \dot{a}_s(\tau) &= A_s a_s(\tau) + F_s(a_s, 0) + B_s u(\tau) \\ u_{\min} &\leq u_i(\tau) \leq u_{\max}, \quad i = 1, 2 \\ \chi^{\min} &\leq C_s a_s(\tau) \leq \chi^{\max}, \quad \tau \in [t, t + T] \end{aligned} \quad (28)$$

where $C_s = [\phi_1(z_c) \phi_2(z_c)]$ is a row vector. We now proceed with the implementation of the predictive control formulation of Eqs. (27) and (28) and choose $q_s = 1000$, $R = rI$, with

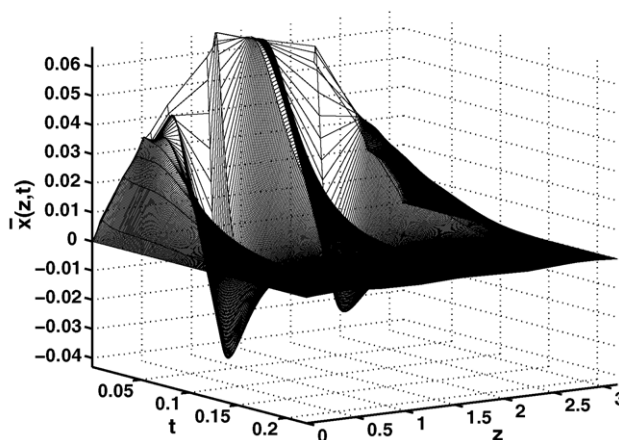


Fig. 2. Closed-loop state profile under the MPC formulation of Eqs. (23) and (24) without accounting for the fast modal states in the constraints.

$r = 0.001$, and $T = 0.011$. In all simulation runs, we considered the following initial condition: $\bar{x}(z, 0) = 0.08 \sin(z) + 0.001 \sin(2z)$ and l is chosen to be 30. The resulting program is solved using the MATLAB subroutine `fmincon`. The control action is then implemented on the 30th order model of Eq. (25). The closed-loop state and manipulated input profiles under the MPC controller of Eqs. (23) and (24) are shown in Figs. 2, 6 and 7 (solid lines), respectively. It is clear that the controller successfully stabilizes the state at the zero steady-state. However, by examining Fig. 5 (solid line), we observe that the state at $z_c = 1.156$ violates the lower constraint for some time. The violation of the state constraint is a consequence of neglecting the contribution of the a_f states to the full state of the PDE in the MPC formulation.

Remark 2. Note that while the controller is designed only on the basis of the slow modes, the stabilization of the slow modes of the system leads to the stabilization of the infinite dimensional system, since the remaining fast modes are open loop stable (for a similar result in the context of linear parabolic PDE systems, see Dubljevic et al., submitted for publication).

Remark 3. For linear parabolic PDEs, low order predictive controller formulations can be derived, which, upon being feasible, guarantee stabilization and state constraint satisfaction of the infinite dimensional system (see, Dubljevic et al., submitted for publication). The inherent coupling between the fast and slow subsystems through the terms $F_s(x_s, x_f)$, $F_f(x_s, x_f)$, however, significantly complicates the derivation of similar results in the nonlinear setting.

Remark 4. State constraints arise either due to the necessity to keep the process state variables within acceptable ranges, to avoid, for example, runaway reactions (in which case they need to be enforced at all times, and treated

as hard constraints) or due to the desire to maintain them within desirable bounds dictated by performance considerations (in which case they may be relaxed, and treated as soft constraints). In the formulations presented in this work, we consider state constraints that need to be enforced at all times, and treated as hard constraints; for predictive controller formulations where the constraints are handled as soft and/or hard constraints, see, e.g., (Mhaskar, El-Farra, & Christofides, in press; Scokaert & Rawlings, 1999).

2.5. Higher-order predictive control formulation

In order to account for the evolution of the fast states in the optimization problem, we consider the following MPC formulation with the objective function and constraints given by:

$$\min_u \int_t^{t+T} [q_s \|x_s(\tau)\|_2^2 + |u(\tau)|_R^2] d\tau \quad (29)$$

$$\begin{aligned} \text{s.t. } \dot{x}_s(\tau) &= A_s x_s(\tau) + \mathcal{F}_s(x_s(\tau), x_f(\tau)) + B_s u(\tau) \\ \dot{x}_f(\tau) &= A_f x_s(\tau) + \mathcal{F}_f(x_s(\tau), x_f(\tau)) + B_f u(\tau) \\ u_{\min} &\leq u_i(\tau) \leq u_{\max}, \quad i = 1, 2 \\ \chi^{\min} &\leq (r, x_s(\tau) + x_f(\tau)) \leq \chi^{\max} \end{aligned} \quad (30)$$

where $\tau \in [t, t + T]$. Note that even though the fast modes appear explicitly in the state constraint equation, they do not appear in the cost function, keeping the computational requirement relatively low.

The MPC formulation above, when written using modal amplitudes, takes the following form:

$$\min_u \int_t^{t+T} [q_s |a_s(\tau)|^2 + |u(\tau)|_R^2] d\tau \quad (31)$$

$$\begin{aligned} \text{s.t. } \dot{a}_s(\tau) &= A_s a_s(\tau) + F_s(a_s(\tau), a_f(\tau)) + B_s u(\tau) \\ \dot{a}_f(\tau) &= A_f a_s(\tau) + F_f(a_s(\tau), a_f(\tau)) + B_f u(\tau) \\ u_{\min} &\leq u_i(\tau) \leq u_{\max}, \quad i = 1, 2 \\ \chi^{\min} &\leq C_s a_s(\tau) + C_f a_f(\tau) \leq \chi^{\max} \end{aligned} \quad (32)$$

where $\tau \in [t, t + T]$, $C_f = [\phi_3(z_c) \cdots \phi_{30}(z_c)]$ is a row vector and the MPC tuning parameters have the same values used in the previous formulation.

Figs. 3 and 5 (dotted lines) demonstrate that the MPC formulation of Eqs. (31) and (32) successfully stabilizes the state profile at the zero steady-state and that the state constraints are satisfied for all times. The corresponding manipulated input profiles are given in Figs. 6 and 7.

Remark 5. Note that even though the optimization problem is nonconvex, and the solution obtained may only represent a local minimum, it does not detrimentally affect the task of state constraint satisfaction, because state constraints are posed as explicit constraints in the optimization problem.

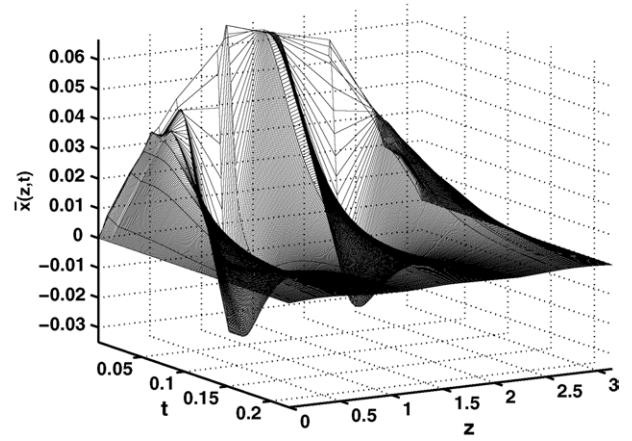


Fig. 3. Closed-loop state profile under the MPC formulation of Eqs. (31) and (32) accounting for the fast modes in the state constraints.

Even if a solution is not a global minimum (which, in general it will not be), the feasibility of the constraints in the optimization problem ensure that upon implementation of this control action, the state constraints will be satisfied for the infinite dimensional system.

Remark 6. Performance considerations can often be expressed as constraints on the state variables. The reduced order MPC formulations, while achieving suboptimal solutions compared to the infinite dimensional optimal control problem (which may not be even computable), can satisfy the performance requirement through satisfaction of the state constraints. Furthermore, while it is not possible to quantify how suboptimal the solution obtained via the reduced order formulation is (due to the inability to compute the solution for the infinite dimensional problem), the optimality properties (with respect to the infinite dimensional problem) can be improved by including more modes in the reduced order formulation.

2.6. High-order predictive control formulation based on two-time-scale approximation

As evidenced by the examples shown before, accounting for the evolution of the fast modes is important for the purpose of satisfying state constraints. The computational complexity associated with accounting for the fast modes could be eased by approximating the dynamics of the fast modes, while retaining the nonlinear dynamics of the slow modes (so as to not adversely effect the task of stabilization). One possible way of approximation is to neglect the nonlinearity in the equations describing the evolution of the fast modes. This is because the term A_f behaves like $1/\epsilon$, where ϵ is a small parameter, and therefore, A_f is much larger than F_f and thus F_f can be neglected from the equation (see Christofides, 2001 for more discussion and analysis of this approximation). Using this approximation, the predictive control formulation takes

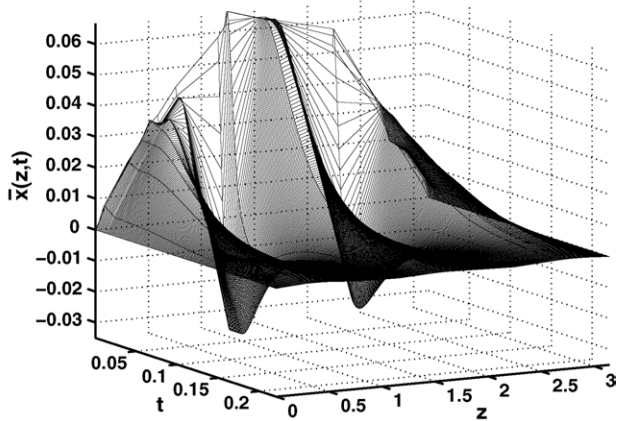


Fig. 4. Closed-loop state profile under the MPC formulation of Eqs. (33) and (34) accounting for the fast modes in the state constraints.

the following form:

$$\min_u \int_0^{t_f} [q_s |a_s(\tau)|^2 + |u(\tau)|_R^2] d\tau \quad (33)$$

$$\begin{aligned} \text{s.t. } \dot{a}_s(\tau) &= A_s a_s + F_s(a_s(\tau), a_f(\tau)) + B_s u(\tau) \\ \dot{a}_f(\tau) &= A_f a_f(\tau) + B_f u(\tau) \\ u_{\min} &\leq u_i(\tau) \leq u_{\max}, \quad i = 1, 2 \\ \chi^{\min} &\leq C_s a_s(\tau) + C_f a_f(\tau) \leq \chi^{\max} \end{aligned} \quad (34)$$

Figs. 4 and 5 (dotted lines) demonstrate that the MPC formulation of Eqs. (33) and (34) successfully stabilizes the state profile at the zero steady-state and that the state constraints are satisfied for all times. The corresponding manipulated input profiles are given in Figs. 6 and 7. Note also, that using the approximations leads to substantial ease in the computational burden and the time required for the computation of the control moves decreases by about 50%.

3. Predictive control of convection-reaction processes

We consider a convection-reaction process example described by the following hyperbolic first-order PDE system:

$$\frac{\partial x_1}{\partial t} = -\frac{\partial x_1}{\partial z} + Da(1 - x_1)e^{x_2/(1+x_2/\gamma)}$$

$$\frac{\partial x_2}{\partial t} = -\frac{\partial x_2}{\partial z} + BDa(1 - x_1)e^{x_2/(1+x_2/\gamma)} + \beta_U(\chi_{w,n} - x_2) + \beta_U \sum_{i=1}^m b_i(z)u_i(t) \quad (35)$$

$$x_1(0, t) = x_1(t), \quad x_2(0, t) = x_2(t), \quad x_1(z, 0) = \bar{x}_1(z), \\ x_2(z, 0) = \bar{x}_2(z)$$

where x_1 denotes a dimensionless conversion, and x_2 denotes a dimensionless temperature, Da is the Damköhler number, γ is a dimensionless activation energy, $\chi_{w,n}$ is the nominal dimensionless wall temperature, B is a dimen-

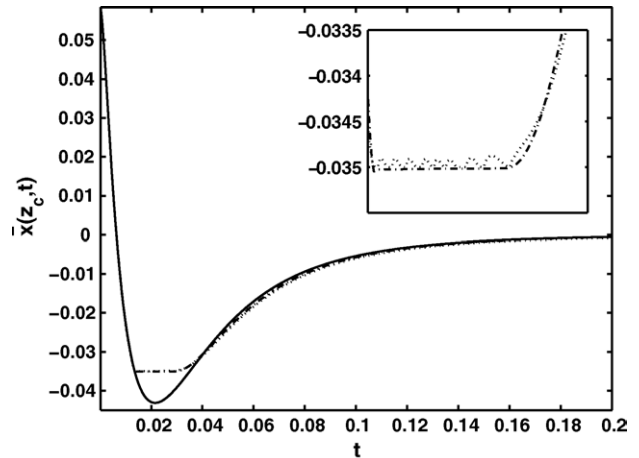


Fig. 5. Closed-loop state profile at $z_c = 1.156$ under the MPC formulation of Eqs. (23) and (24) without accounting for the evolution of fast modes (solid), under the MPC formulation of Eqs. (31) and (32) accounting for the fast modes in the state constraints (dotted), and under the MPC formulation of Eqs. (33) and (34) using linearization approximation for the evolution of modal states in the constraints (dashed-dotted).

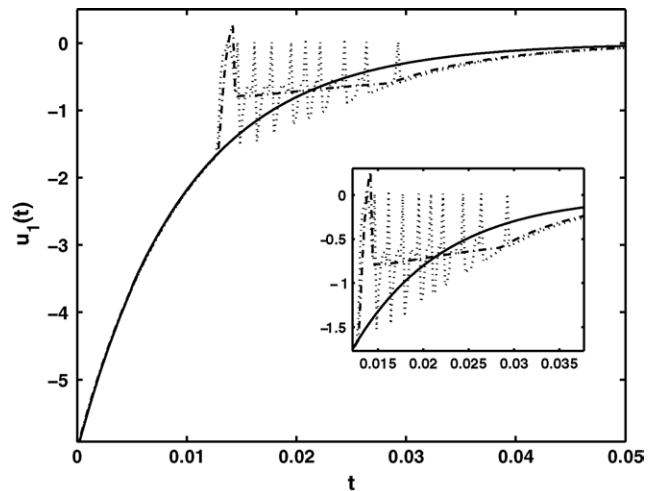


Fig. 6. Manipulated input profiles for the first control actuator applied at $z_{a1} = \pi/3$ under the MPC formulation of Eqs. (23) and (24) (solid), under the MPC formulation of Eqs. (31) and (32) (dotted), and under the MPC formulation of Eqs. (33) and (34) (dashed-dotted).

sionless heat of reaction, β_U denotes a dimensionless heat transfer coefficient, $u_i(t)$ denotes change in wall temperature from the nominal value and is the manipulated input, and $b_i(z)$ is the distribution function of the i th actuator, cho-

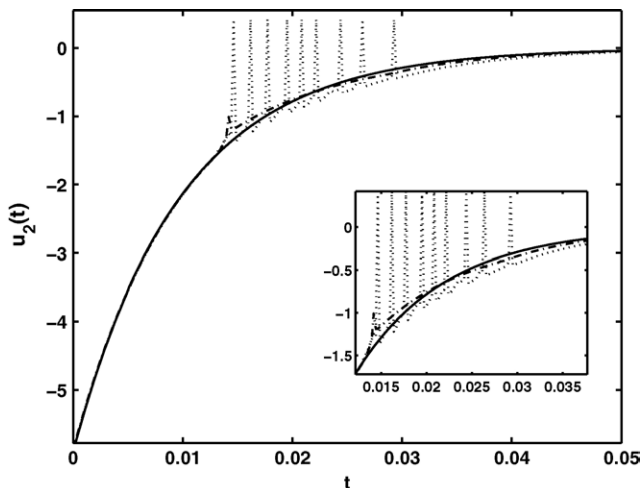


Fig. 7. Manipulated input profiles for the second control actuator applied at $z_{a2} = 2\pi/3$ under the MPC formulation of Eqs. (23) and (24) (solid), under the MPC formulation of Eqs. (31) and (32) (dotted), and under the MPC formulation of Eqs. (33) and (34) (dashed-dotted).

sen to be $b_i(z) = [H(z - z_i) - H(z - z_{i+1})]$ where $H(z)$ is the standard Heaviside function. The following typical values are given to the process parameters: $Da = 0.25$, $B = 10.5$, $\beta_U = 5.4$, $\chi_{w,n} = 0.1$ and $\gamma = 8$. The initial conditions chosen were $\bar{x}_1(z) = \bar{x}_2(z) = 0$, and the boundary conditions were chosen to be $x_1(t) = 0.05$ and $x_2(t) = 4.0$. For these values, it was verified that the operating steady-state profile is stable (solid lines in Fig. 8 depict the steady state profile of the temperature T in the reactor). The dashed lines

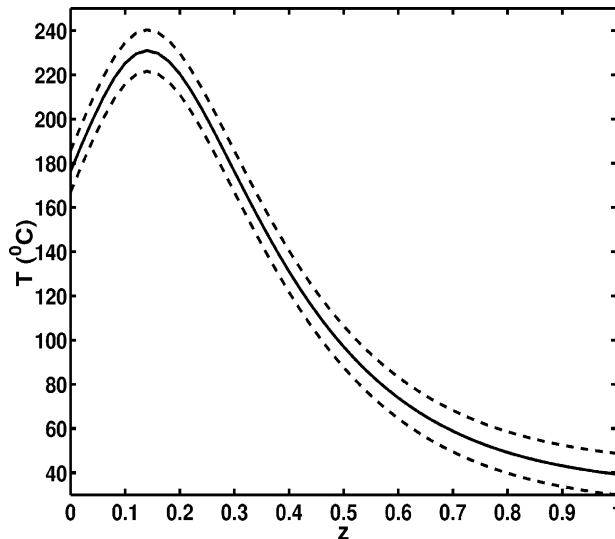


Fig. 8. Open-loop profile showing the steady-state temperature profile (solid lines). The dashed lines denote the upper and lower constraints on the temperature.

Note that reducing the value of $x_1(t)$ implies greater inlet reactant concentration, increased reaction and heat generation in the reactor, that subsequently leads to violation of the state constraints in the reactor.

We therefore consider the control objective of maintaining the desired steady-state profile along the reactor within the bounds of allowed temperature variation in the presence of disturbances. A predictive control algorithm, designed to achieve the aforementioned control objective takes the following form:

$$\begin{aligned}
 \min_{u(\tau)} & \int_t^{t+T} \left[\left\{ \int_Z e(z, \tau)^2 q \, dz \right\} + u' Ru \right] d\tau \\
 \text{s.t.} & \quad \frac{\partial x_1}{\partial t} = -\frac{\partial x_1}{\partial z} + Da(1 - x_1) e^{x_2/(1+x_2/\gamma)} \\
 & \quad \frac{\partial x_2}{\partial t} = -\frac{\partial x_2}{\partial z} + BDa(1 - x_1) e^{x_2/(1+x_2/\gamma)} + \beta_U(\chi_{w,n} - x_2) + \beta_U \sum_{i=1}^m b_i(z)u_i(t) \quad (36) \\
 & \quad x_1(0, t) = x_1(t), \quad x_2(0, t) = x_2(t), \quad x_1(z, 0) = \bar{x}_1(z), \quad x_2(z, 0) = \bar{x}_2(z) \\
 & \quad u_i^{\min} \leq u_i \leq u_i^{\max}, \quad i = 1, \dots, m \\
 & \quad x_{2\min} \leq x_2(z, t + \tau) \leq x_{2\max} \forall z \in Z, \tau \in [t, t + T]
 \end{aligned}$$

represent constraints on the temperature in the reactor and correspond to the constraints in the dimensionless state variable given by $x_2^{\max} = x_{2s} + 0.25$, $x_2^{\min} = x_{2s} - 0.25$.

Due to the exothermic nature of the reaction, a small increase/decrease in the inlet concentration may result (by changing the net reaction, and therefore, the net heat generation) in a significant change in the peak of the temperature profile in the reactor (see dash-dotted line in Fig. 9 for the steady-state profile in the reactor under the presence of a negative disturbance of magnitude 0.03 in both $x_1(t)$ and $x_2(t)$).

where $e(z, \tau) = x_{2ss} - x_2(z, \tau)$, $u_i^{\max}, u_i^{\min}, i = 1, \dots, m$ represent constraints on the manipulated variables, and x_2^{\min}, x_2^{\max} represent state constraints. The above optimization problem may be solved off-line or solved in a receding horizon fashion and implemented online in order to achieve robustness of the closed-loop system with respect to unknown disturbances.

The PDE system of Eq. (35) being hyperbolic, however, prevents the use of low-order approximations that can be used for the purpose of controller design, and renders the task of real-time implementation of the controller design of Eq. (36), or of quantifying the loss in optimality when implementing

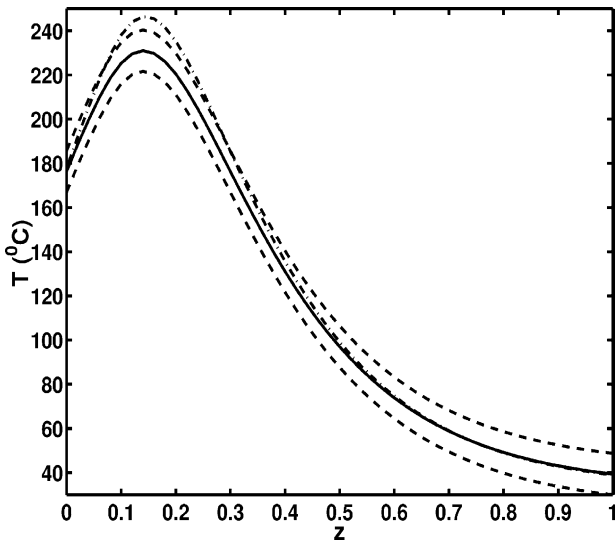


Fig. 9. The steady-state temperature profile (dash-dotted lines) induced by a negative disturbance of magnitude 0.03 in the dimensionless inlet temperature and concentration.

an approximation, very difficult. To come up with a controller design that can be readily implemented in real time, we make the following simplifications: first, we exploit the fact that for the system under consideration, the transients are very fast, and both the control objective, and the state constraint satisfaction can be required to hold at the steady-state. Then, to reduce the complexity of the computation, the decision variable is chosen as a feedback gain, instead of the manipulated inputs themselves. Finally, instead of requiring the constraints to hold over the entire spatial domain, we restrict it to a zone, and furthermore, divide the zone into a number of subzones, such that in each subzone, a different value of the control action can be implemented. Specifically, we solve the following optimization problem:

$$\min_K \left[\left\{ \int_{\Delta Z} q e_s(z)^2 dz \right\} + u'_s R u_s \right]$$

$$\text{s.t. } 0 = -\frac{\partial x'_{1s}}{\partial z} + Da(1 - x'_{1s}) e^{x'_{2s}/(1+x'_{2s}/\gamma)}$$

$$0 = -\frac{\partial x'_{2s}}{\partial z} + BDa(1 - x'_{1s}) e^{x'_{2s}/(1+x'_{2s}/\gamma)} + \beta_U (\chi_{w,n} - x'_{2s}) + \beta_U \sum_{i=1}^2 b_i(z) u_{is}$$

$$x'_{1s}(0) = x_{1d}, \quad x'_{2s}(0) = x_{2d}$$

$$u_{i,s} = K_i \frac{\int_{\Delta Z_i} e_s(z) dz}{\Delta Z_i}$$

$$u_i^{\min} \leq u_{is} \leq u_i^{\max}, \quad i = 1, \dots, m$$

$$x_2^{\min} \leq x'_{2s}(z) \leq x_2^{\max} \forall z \in \Delta Z$$

where $K = [K_i], i = 1, \dots, m$, are the gains that multiply the error, $e_s(z) = x'_{2s} - x_{2s}$, where x_{2s} is the ‘unperturbed’, open-loop steady-state profiles, x'_{2s} is the closed-loop steady-state profiles, and $\Delta Z_i, i = 1, \dots, m$ denote the subzones within the control zone, x_{1d} and x_{2d} represent the steady-state inlet concentration and temperature, respectively.

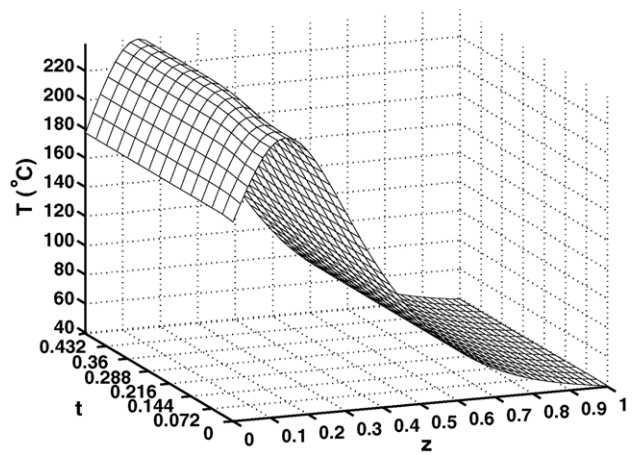


Fig. 10. Closed-loop evolution of the temperature profile in the presence of disturbance.

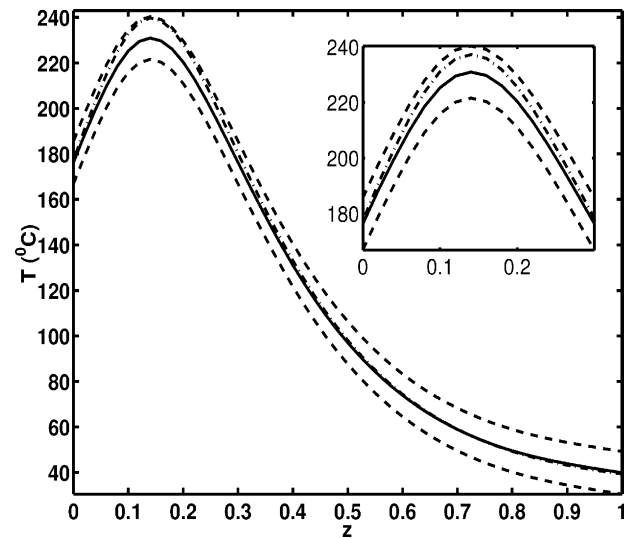


Fig. 11. Steady state closed-loop profile (dash-dotted line) in the presence of disturbance.

$$(37)$$

In the simulation results, the control zone is chosen to be $\Delta Z \in [0.04, 0.3]$ and divided into three subzones. The finite-difference method is used for the integration of the hyperbolic PDE with discretization in space $\delta z = 0.02$, and with explicit Newton integration in time with $\delta t = 0.0001$. The parameters in the objective function of Eq. (37) were chosen as $q = 20, R = rI, r = 0.001, x_2^{\max} = x_{2s} + 0.25, x_2^{\min} = x_{2s} - 0.25, u^{\min} = -2$ and $u^{\max} = 2$. Figs. 10 and 11 demonstrate that the controller successfully achieves state constraint satisfaction and drives the

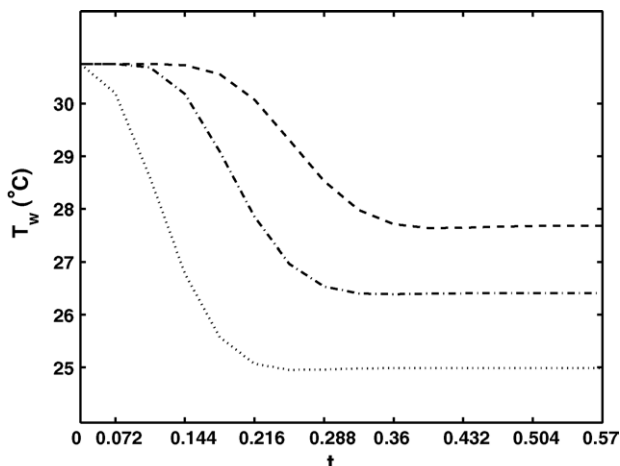


Fig. 12. Dotted, dash-dotted, and dashed lines represent the evolution of the wall temperature, T_w , in the control zones 1, 2 and 3, respectively.

closed-loop state profile (dash-dotted lines) close to the desired state profile. Note that in the absence of control, the state constraints are violated in the presence of disturbance (see Fig. 9).

4. Conclusions

In summary, this work focussed on the development of computationally efficient predictive control algorithms for nonlinear parabolic and hyperbolic PDEs with state and control constraints arising in the context of transport-reaction processes. We first considered a diffusion-reaction process described by a nonlinear parabolic PDE and addressed the problem of stabilization of an unstable steady-state subject to input and state constraints. Galerkin's method was used to derive finite-dimensional systems that capture the dominant dynamics of the parabolic PDE, which were subsequently used for controller design. Various MPC formulations were constructed on the basis of the finite dimensional approximations and were demonstrated, through simulation, to achieve the control objectives. We then considered a convection-reaction process example described by a set of hyperbolic PDEs and addressed the problem of stabilization of the desired steady-state subject to input and state constraints, in the presence of disturbances. An easily implementable predictive controller based on a finite dimensional approximation of the PDE obtained by the finite difference method was derived and demonstrated, via simulation, to achieve the control objective (Fig. 12).

Acknowledgement

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