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MODEL PREDICTIVE CONTROL OF DIFFUSION-REACTION PROCESSES

Parabolic partial differential equations naturally arise as an adequate representation of a large class of spatially distributed systems, such as diffusion–reaction processes, where the interplay between diffusive and reaction forces introduces complexity in the characterization of the system, for the purpose of process parameter identiffcation and subsequent control. In this work we introduce a model predictive control (MPC) framework for the control of input and state constrained parabolic partial differential equation (PDEs) systems. Model predictive control (MPC) is one of the most popular control formulations among chemical engineers, manly due to its ability to account for the actuator (input) constraints that inevitably exist due to finite actuator power and its ability to handle state constraints within an optimal control setting. In controller synthesis, the initially parabolic partial differential equation of the diffusionreaction type is transformed by the Galerkin method into a system of ordinary differential equations (ODEs) that capture the dominant dynamics of the PDE system. Systems obtained in such a way (ODEs) are used as the basis for the synthesis of the MPC controller that explicitly accounts for the input and state constraints. Namely, the modified MPC formulation includes a penalty term that is directly added to the objective function and through the appropriate structure of the controller state constraints accounts for the infinite dimensional nature of the state of the PDE system. The MPC controller design method is successively applied to control of the diffusion–reaction process described by linear parabolic PDE, by demonstrating stabilization of the non–dimensional temperature profile around a spatially uniform unstable steady–state under satisfaction of the input (actuator) constraints and allowable non–dimensional temperature (state) constraints.

Key words: Parameter distributed systems, Galerkin method, Input/ /output/state constraints, Model predictive control (MPC).

Transport–reaction processes are characterized by wide spatial variations due to underlying diffusion and transport phenomena the model descriptions of which are given by non–linear parabolic partial differential equations (PDEs). Process operation specifications often require that the states of the system be maintained within certain bounds, therefore any appropriate control design for such process specifications needs to take into account the spatial nature of the process and to enforce state constraints while respecting those constraints on the manipulated inputs arising due to physical limitations in the functioning of the control actuators.

The modelling of transport–reaction processes in finite spatial domains naturally yields parabolic PDE systems that have spatial differential operators the spectrum of which can be partitioned into a finite (possibly unstable) slow part and an infinite stable fast complement. Therefore, the traditional approach to the control of parabolic PDEs involves the application of spatial discretization techniques to the PDE system to derive large systems of ordinary differential equations (ODEs), that accurately describe the dynamics of the dominant (slow) modes of the PDE system. These are subsequently used as the basis for the synthesis of finite–dimensional controllers (e.g., [3,5,11]) where a finite, typically small, number of controll actuators ($u_i(t)$) and measurement sensors ($y_m^i(t)$) are used to control the spatially distributed state ($y_c^i(t)$) (see Fig. 3). Issues such as the output/state and input constraints very naturally bring Model Predictive Control (MPC) into consideration as a control methodology for handling constraints within an optimal control setting. In MPC, the control action is achieved through a finitešhorizon constrained open–loop optimal control problem, which results in a linear program (LP) or quadratic program (QP) and which is solved repeatedly at each sampling time with constraints explicitly accounted as constraints on the LP/QP. In other words, the MPC uses a process model to predict a future trajectory, and then computes a future trajectory that optimizes the performance objective, based on the model prediction. One reason for the popularity of the MPC is its ability to directly include constraints in the computation of the control input. Usually, the introduction of "hard" – input constraints does not pose a problem, while at the same time, the satisfaction of the "soft" – state and output constraints is more dificult. Thereby, a combination of the actuator, state and output constraints can potentially lead to infeasibility in the LP/QP. One possible formulation to handle the state and output constraints is a "soft constraints" formulation, in which penalty terms on the constraints are included in the objective function [6,8,12]. The soft constraint approach avoids infeasibility of the constrained optimization problem by allowing the state and output constraints to be violated, but penalizes constrained violation by placing sufficiently large

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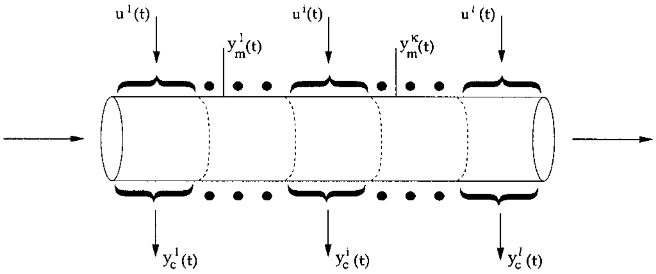

Figure 1. Control problem specifications for a plug reactor

penalties on the constraints violation in the objective functional.

The traditional approach to the control of a parabolic PDE within the MPC framework, where a potential drawback of using spatial discretization techniques 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 an MPC controller design that is highly computation–intensive. Recent advances in model reduction techniques have made tools like Galerkin's method available (either through analytical or through data–based construction of the basis functions) which yields low order ODE models, capable of capturing the behavior of the system accurately enough to be useful for the purpose of the controller design (e.g., see [1,2,7] and the book [4] for results and references in this area).

Motivated by these considerations, we develop, in this work, a framework to exploit the input and state constraints handling and optimality properties of a model predictive controller for the stabilization of linear parabolic PDEs. The MPC controller is designed on the basis of a lower order model obtained through the Galerkin's method, and the objective function in the optimization problem is enlarged for the appropriate penalty terms associated with the higher modes of the PDE. The input constraints are handled directly through the MPC controller, while the state constraints are handled via constraints on the states of the lower order system, which are corrected for the time–dependent evolution of the higher modes of the PDE. Handling both state and input constraints through the optimization algorithm that accounts for the constraints being not violated on the sifnificantly large finite dimensional approximation of the entire state, links the infinite dimensional nature of the state of the parabolic partial differential equation with the best performance and optimality characteristics of MPC design.

1. PRELIMINARIES

1.1. Parabolic infinite dimensional systems

In this work, we focus on the control of linear parabolic PDEs of the form:

$$\frac{\partial \bar{x}}{\partial t} = b\frac{\partial^2 \bar{x}}{\partial z^2} + \omega \sum_{i=1}^{m} b_i(z)u_i + \alpha\bar{x} \qquad (1)$$

subject to the boundary conditions:

$$\bar{x}(0,t) = 0, \quad \bar{x}(\pi,t) = 0 \qquad (2)$$

and the initial condition:

$$\bar{x}(z,0) = \bar{x}_0(z) \qquad (3)$$

where $\bar{x}(z,t) \in \mathrm{IR}$ denotes the state variable, $z \in [0,\pi] \subset \mathrm{IR}$ is the spatial coordinate, $t \in [0,\infty]$ is the time, $u_i \in \mathrm{IR}$ denotes the i–th constrained manipulated input; u_i^{min} and u_i^{max} are real numbers representing, respectively, the lower and upper bounds on the i–th input, and χ^{min} and χ^{max} are real numbers. The term $\frac{\partial^2 \bar{x}}{\partial z^2}$ denotes the second–order spatial derivative of $\bar{x}$; α, b and ω are constant real numbers with b>0, and $\bar{x}(z)$ is a suficiently smooth function of z. The function $b_i(z)$ is a known smooth function of z that describes how the control action, $u_i(t)$, is distributed in the finite interval $[0,\pi]$. Whenever the control action enters the system at a single point z_a, with $z_a \in [0,\pi]$ (i.e., point actuation), the function $b_i(z)$ is taken to be non–zero in a finite spatial interval of the form $[z_a - \mu, z_a + \mu]$, where μ is a small positive real number, and zero elsewhere in $[0,\pi]$. The function r(z) is a "state constraints distribution" function that describes where the state constraints are to be enforced in the spatial domain, $[0,\pi]$. With no need for the introduction of a detailed mathematical description, we use x'Qx to denote a weighted norm, where Q is a positive–definite matrix and x' denotes the transpose of x.

2. MODEL PREDICTIVE CONTROL FORMULATIONS

It is known that within the framework of the model predictive control (MPC) of finite dimensional systems, the crucial issue of the input and output/state constraints can be adequately addressed in the explicit manner. However, when it comes to spatially distributed systems, it is necessary to account for the infinite dimensional nature of the state of the PDE (i.e., a non–dimensional temperature $\bar{x}(z,t) = \sum_{i=1}^{\infty} x_i(t))$, which requires MPC controller design that will incorporate state constraints in the adequate manner. Namely, state constraints are given as limits on the state:

$$\chi^{min} \le (r(z), \bar{x}(z,t)) \le \chi^{max} \qquad (4)$$

where r(z) is the state constraint distribution function that determines where the constraints are active in the spatial domain. For example, state constraints over a spatial domain are such that they may require in a certain spatial region that the state is kept within defined limits (e.g. in the region close to the boundary of the domain, due to reasons of safety or other performance

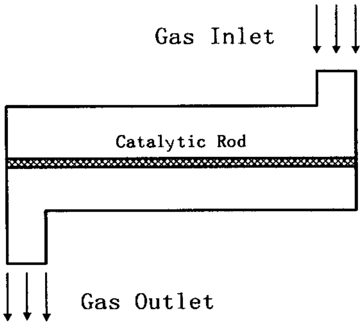

Figure 2. Catalytic rod reactor

requirements, a non–dimensional temperature should not exceed a certain limit). In particular, the PDE state constraints are appropriately expressed as constraints on the modal states, assuming that for the sake of demonstration of the proposed methodology, the number of x_f (t) – "fast" modal states taken into account in a high–order approximation of the infinite–dimensional PDE is large but still finite, allowing us to construct a finite horizon optimal constrained optimization problem.

2.1. MPC formulations: accounting for the input and state constraints

In the MPC algorithm, we consider model predictive control of the system described by the discrete version of Eq1. 1–3 (see Appendix 1 and 2 for detailed derivation of Eq. (k))

$$\begin{aligned} x_s(k+1) &= F_s x_s(k) + G_s u(k) \\ x_f(k+1) &= F_f x_f(k) + G_f u(k) \\ x_s(0) &= x_{s0}, \quad x_f(0) = x_{f0}, \quad k = 0,1,... \end{aligned} \tag{5}$$

subject to the control and output constraints,

$$\begin{aligned} u_j^{min} &\le u_j(k) \le u_j^{max} \quad j = 1,2,...,l \\ \chi_g^{min} &\le Cx(k) \le \chi_g^{max} \quad g = 1,2,...,p \end{aligned} \tag{6}$$

where j represents a number of actuators and p represents a number of measurement sensors applied along the spatial domain with corresponding values for the input and state constraints enforced at those locations. For a given time k, the MPC controller solves a constrained optimization problem:

$$\min_u \sum_{i=0}^{N-1} \{[x(k+i)'Qx(k+i)+u(k+i)'Ru(k+i)]+ +x(k+N)'\bar{Q}x(k+N)\} \tag{7}$$

$$\begin{aligned} \text{s.t. } x_s(i+1) &= F_s x_s(i) + G_s u(i) \\ x_f(i+1) &= F_f x_f(i) + G_f u(i) \quad i=1,2,...,N-1 \\ u_j^{min} &\le u_j(i) \le u_j^{max} \quad j=1,2,...,l \\ \chi_g^{min} &\le Cx(i) \le \chi_g^{max} \quad g=1,2,...,p \end{aligned} \tag{8}$$

where $x(i) = [x_s(i)\ x_f(i)]$ and $u = [u(i), u(i+1),..., u(i+N-1)]$ is a vector of the control moves computed over the control horizon N, R>0 is a strictly positive definite and

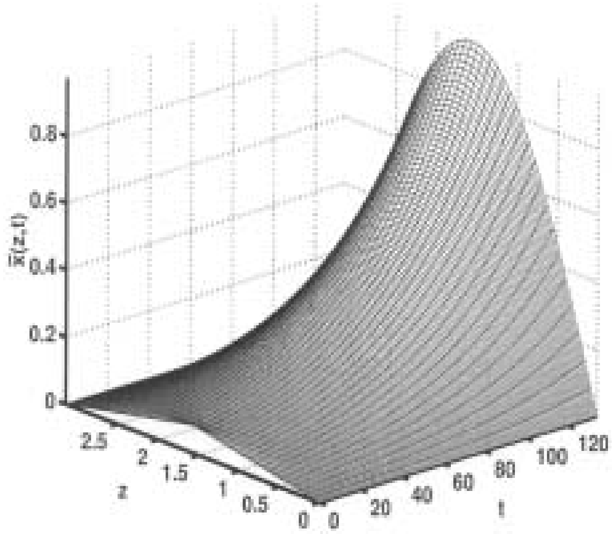

Figure 3. Open–loop temperature profile showing the instability of the x(z,t) = 0 steadystate.

$Q = C'QC \ge 0$ is a positive semidefinite matrix, matrix $\bar{Q}$ denotes a terminal penalty through which the stabilization of the unstable modes is assured at the end of the receding horizon, assuming that the constrained optimization problem, cast as a quadratic programming (QP) [9], provides a feasible solution with respect to the initial conditions $x(0) = (x_s(0), x_f(0))$. Although, the afore-mentioned MPC formulation Eq.7–Eq.8 accounts for the full modal dynamics in the optimization functional Eq.7 and in the constraints Eq.8, a potential drawback is the use of a high–order model describing the evolution of the fast modes that yields a computationally demanding structure of the constrained optimization problem that must be solved at each time instance of the MPC control law implementation (e.i. in real–time in order for it to be possible to be implemented). Therefore, in order to circumvent the high dimensionality of the MPC controller, low–order formulations are proposed.

2.2. Low–order MPC formulations

In the ensuing 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). The MPC controller is obtained by solving the following optimization problem:

$$\min_u \sum_{i=0}^{N-1} \{[x_s(k+i)'Qx_s(k+i)+u(k+i)'Ru(k+i)]+ +x_s(k+N)'\bar{Q}x_s(k+N)\} \tag{9}$$

$$\begin{aligned} \text{s.t. } x_s(i+1) &= F_s x_s(i) + G_s u(i) \quad i=1,2,...,N-1 \\ x_f(i+1) &= F_f x_f(i) + G_f u(i) \\ u_j^{min} &\le u_j(i) \le u_j^{max} \quad j=1,2,...,l \\ \chi_g^{min} &\le C_s x_s(i) \le \chi_g^{max} \quad g=1,2,...,p \end{aligned} \tag{10}$$

Unlike the formulation of Eqs. 7–8, the above formulation includes penalties only on the slow states and the input. The evolution of the fast states is not accounted for in the cost functional nor in the state constraints. Despite its low–order characteristic, a potential drawback of this formulation is the fact that, when appropriate stability constraints are incorporated into the optimization problem, the resulting MPC law, when implemented on the full system of Eq.5, can only enforce closed–loop stability, but not necessarily full–state constraints satisfaction, since it neglects the evolution of the fast states. Therefore, it is necessary to account for the fast mode dynamics in order to satisfy the constraints and still maintain a low–order of the MPC formulation.

2.2.1. Low–order MPC formulations with state constraints

In order to account for the effect of the fast states on the full–state constraints, the formulation of Eqs. 9–10 can be modified by incorporating the fast states into the state constraints equation. The control action in this case is computed by solving the following optimization problem:

$$\min_{u} \sum_{i=0}^{N-1} \{[x_s(k+i)'Qx_s(k+i)+u(k+i)'Ru(k+i)]+ +x_s(k+N)'\bar{Q}x_s(k+N) + \Gamma(x_f)\} \quad (11)$$

$$\text{s.t. } x_s(i+1) = F_s x_s(i) + G_s u(i)$$

$$x_f(i+1) = F_f x_f(i) + G_f u(i) \quad i = 1,2,\ldots,N-1$$

$$u_j^{min} \le u_j(i) \le u_j^{max} \quad j = 1,2,\ldots, l \quad (12)$$

$$\chi_g^{min} \le C_s x_s(i) \le \chi_g^{max} \quad g = 1,2,\ldots,p$$

The constructed predictive control law formulation Eq.11–Eq.12, at each time of the predictive control implementation, solves a constrained optimization program based on the slow mode dynamics, whereas the state constraints are represented in the form of the two contributions, one that is associated with the modal states of the x_s – "slow" dimensional system and another complementary contribution of the x_f – "fast" modes of the system that accounts for the infinite dimensional property of the PDE state. By doing this, the "fast" mode evolution is exactly accounted for and enforced in the construction of the control input based only on the slow subsystem in the MPC control law implementation, so that possible state constraints violation is avoided and ensures that if the MPC optimization problem is initially feasible, it will successfully stabilize the system in a closed–loop, account for the performance criterion and continue to be feasible.

Subsequent feasibility is guaranteed by the claim that there exists a sufficiently long horizon for the feasibility to be achieved and the lenght of the horizon (N) can be computed as given in [10]. A proper account for the influence of the "fast" modal state evolution is twofold, in a sense that it allows us to directly account for them in the state constraints evolution, and also allows the characterization of some appropriate measure of the peaking magnitude of the fast modes and, therefore, explicitly accounts for penalizing the peaking through an added penalty term $\Gamma(x_f)$ in the objective functional Eq.11. The penalty term can admit various forms that can be proposed for quantifying the "fast" modal states peaking, for example, the penalty term can be expressed in the form of the "worst–case" l_∞–norm of the "fast" states peaking within the prediction horizon, or the l_1–norm which is the sum of the overall time steps in the prediction horizon of the absolute value of the predicted fast mode dynamics, and the l_2–norm is the squared sum of the predicted peaking summed over all time steps in the prediction horizon. Usually, the l_∞–norm is a popular choice in order to minimize for the "worst–case" peaking induced by the input control action. Along the same line, an important feature of such employed state constraint in the framework of the parabolic PDEs is that the "fast" modal states of the finite dimensional approximation of Eq.5 are exponentially stable and therefore "fast" mode constraints also vanish, relaxing the "slow" modal state constraints that are present in the MPC optimization algorithm. This feature impinges on the crucial issue of the initial feasibility of the optimization algorithm where stringent requirements on the state constraints can be directly related to the infeasibility of the MPC algorithm.

The function $\Gamma(x_f)$ is the penalty function that increases the optimization criterion when excessive peaking of the higher modes takes place, and it is associated with the vector of the weighted norms l_∞ of the fast mode peaking. The penalty function is given in the most general form as,

$$\Gamma(x_f) = p^T H p + h^T p \quad (13)$$

where matrices H and h are appropriate weights on the peaking penalization of the "fast" modes. The matrix H is assumed to be a positive definite in order to be able to formulate the optimization problem as a standard QP problem, whereas the vector h is assumed not to have negative elements [6]. The vector p is given as an appropriate norm on the evolution of the fast states,

$$p = \|C_f x_f(i)\| \quad (14)$$

where x_f denotes "fast" states that are not taken in the account in the performance function through the weighted evolution of modes, Eq. 11, but through the penalty function. However, it is important to distinguish cases when the evolution of "fast" modes and their peaking is penalized and whether the penalization includes only the contribution to the "fast" state evolution due to the input, or we also account for the fast exponentially stable part of the evolution of the "fast" modes. In that more conservative sense, we penalize peaking that contributes from the inherent dynamics and input induced dynamics of the fast modes. Hence, after being appropriately accounted for the peaking, the "fast" modes die due to the high exponential stability of their intrinsic dynamics after some time provided that the system can initially be stabilized.

Remark 1: The linear structure of Eg.5, where the only source of the coupling between the slow and fast subsystem is given through the control input, implies that the evolution of the slow states, in the closed–loop system, is not dependent upon the fast modes. An important consequence of this fact is that the asymptotic stability obtained on the basis of the slow finite dimensional system Eg.5 would result in the asymptotic stability in an infinite–dimensional closed–loop system.

3. ILLUSTRATIVE EXAMPLE

In this section, we demonstrate by means of computer simulations how the concept of a distributed MPC controller can be used to deal with the problem of constrained stabilization of parabolic PDEs in the presence of the state and input constraints which are due to physical limitations of the actuators and allowable state limitations.

Consider a long, thin rod in a reactor (Figure 3) which is fed with pure species A and a zero–th order exothermic catalytic reaction takes place on the rod. As an exothermic reaction progresses on the rod, a cooling medium that is in contact with the catalytic rod is used for the cooling. Under the assumptions of a constant density and heat capacity of the rod, a constant conductivity of the rod, and constant temperature at both ends of the rod, and an excess of the species A in the feed, the mathematical model which describes the spatiotemporal evolution of the dimensionless rod temperature consists of the following parabolic PDE:

$$\frac{\partial \bar{x}}{\partial t} = \frac{\partial^2 \bar{x}}{\partial z^2} + (\beta_T e^{-\gamma}\gamma - \beta_U)\bar{x} + \beta_U \sum_{j=1}^{n} b_j(z)u_j(t)$$
$$\bar{x}(0,t) = 0,\ \bar{x}(\pi,t) = 0,\ \bar{x}(z,0) = x_0(z) \tag{15}$$

which represents a linearized model of a typical diffusion–reaction process, around the zero steady–state, where $\bar{x}$ denotes a dimensionless temperature, 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 corresponding 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 demonstrated in Fig. 3 which shows the evolution of the open–loop rod temperature starting from initial conditions close to the steady state $\bar{x}(z,t) = 0$, so that the process moves to another stable steady state characterized by a maximum in the temperature profile, a "*hot–spot*" in the middle of the rod. The control objective is to stabilize the state profile at the unstable zero steady–state by manipulating the $u_i(t)$ subject to the following input and state constraint

$$u_i^{min} \le u_i \le u_i^{max} \tag{16}$$

$$\chi^{min} \le \int_0^{\pi} r(z)\bar{x}(z,t)dz \le \chi^{max} \tag{17}$$

where $u_i^{min} = -4$, $u_i^{max} = 4$, for i=1,2, $\chi^{min} = -0.025$, $\chi^{max} = 2$. The state constraints distribution function, $r(\cdot)$, is chosen to be $r(z) = \delta(z-z_{cj})$, where j=1,...,p is a number of available (pointwise) measurements, which implies that the state constraints are to be enforced at a single point in the spatial domain, i.e., $-0.025 \le \bar{x}(z_{cj},t) \le 2$.

The eigenvalue problem for the spatial differential operator of the PDE of Eq.35 can be solved analytically and its solution yields,

$$\lambda_j(z) = 1.66 - j^2,\quad \phi_j(z)= \sqrt{\frac{2}{\pi}}\sin(jz),\quad j=1,...,\infty \tag{18}$$

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. 16–17. To simplify the presentation of the results, we will work with the amplitudes of the eigenmodes of the PDE of Eq.1. Specifically, by using standard modal decomposition, we derive the following high–order discrete ODE system that describes the temporal evolution of the amplitudes of the first eigenmodes:

$$a_s(k+1) = A_s a_s(k) + B_s u(k)$$
$$a_f(k+1) = A_f a_f(k) + B_f u(k)\quad k = 0,1,... \tag{19}$$

where $a_s(k) = [a_1(k)\ a_2(k)]'$, $a_f(k) = [a_3(k)\ a_4(k)\ ...\ a_l(k)]'$, $a_i(k) \in IR$ is the modal amplitude of the i–th eigenmode, the notation a_s' denotes the transpose of a_s, $u(k) = [u_1(k)\ u_2(k)]'$, the matrices A_s and A_f are diagonal matrices, given by $A_s = diag\{\lambda_i\}$, for i=1,2 and $A_f = diag\{\lambda_i\}$, for i=3,...,l. B_s and B_f are a 2x2 and (l–2) x m matrices, respectively, whose (i,j)–th element is given by $B_{ij}=(b_j(z), \phi_i(z))$. Note, that $\bar{x}(z,t) = \sum_{i=1}^{l} a_i(k)\phi_i(z)$, $x_s(k) = a_1(k)\phi_1 + a_2\phi_2$, $x_f(k) = \sum_{i=3}^{l} a_i(k)\phi_i$, and that $(x_s(k),\phi_i) = = a_i(k)(\phi_i,\phi_i)$. Using these projections, the state constraints of Eq.17

can be expressed as constraints on the modal amplitudes as follows:

$$\chi^{min} \le \sum_{i=1}^{2} a_i(k)\phi_i(z_{cj}) + \sum_{i=3}^{l} a_i(k)\phi_i(z_{cj}) \le \chi^{max} \quad (20)$$

where points where state constraints are forced are given as follows,

$$z_{cj} = [0.0682\ \ 0.2919\ \ 0.4244\ \ 0.5011\ \ 0.5875\ \ 0.7574\ \ 1.0472\ \ 1.2287\ \ 1.5067\ \ 1.6063\ \ 2.0944\ \ 2.2368\ \ 2.6531\ \ 2.7376\ \ 2.7621\ \ 2.9138\ \ 3.0828] \quad (21)$$

We now proceed with the implementation of different predictive controller formulations presented in Section 2.2. The following initial condition is considered in all the simulation results $\bar{x}(z,0)=0.04\ \sin(z)$ and approximation of the state of infinite dimensional PDE is realized by taking l=30. In the first considered scenario, the low dimensional MPC formulation, at each time step i, is based on two–slow modes in the performance functional and in the state constraints:

$$\min_{u} \sum_{k=0}^{N-1} \{[a_s(k+i)'Qa_s(k+i)+u(k+i)'Ru(k+i)]+ +x_s(i+N)'\bar{Q}x_s(i+N)\} \quad (22)$$

$$\text{s.t. } a_s(k+1) = A_s a_s(k) + B_s u(k) \quad k=0,1,2,..., N-1$$
$$u_j^{min} \le u_j(k) \le u_j^{max} \quad j=1,2 \quad (23)$$
$$\chi_g^{min} \le C_s x_s(k) \le \chi_g^{max} \quad g=1,2,...,p$$

where with $Q = C_s' Q C_s$, with $C_s = [\phi_1(z_{cj})\ \phi_2(z_{cj})]$ and the appropriate weights Q=30 and R=Ir, with r=0.001, with the horizon lenght N=100 and state constraints are enforced at p=17 points along the spatial domain Eq.21. In order to ensure stability, the terminal equality constraint on the slow–modes, i.e. $a_s(i+N)=0$, is included in the receding horizon problem Eqs. 22–23. The above receding constrained horizon problem is solved using the MATLAB subroutine QuadProg.

Remark 2: In order to obtain a discrete description of Eq.19 from the continuous description of Eq.15 (see Appendix 2), a standard transformation is applied with the sampling time γ, defined as $\delta = \dfrac{1}{2\max|\{\sigma(A)\}|}$.

The control action computed on the basis of the constrained optimization problem Eqs.22–23 when applied to the 30–th order model of Eq.19. Fig.4 and Figs.7–8 show that the MPC controller successfully stabilizes a spatially uniform unstable steady–state $\bar{x}(z,t)=0$. However, we observe that the state constraints are severely violated along the spatial domain in the vicinity of the points of actuator implementation, respectively $z_{c1}=\pi/3$ and $z_{c2}=2\pi/3$. In order to guarantee state constraints satisfaction and closed–loop stability, still having low–order MPC formulation, we

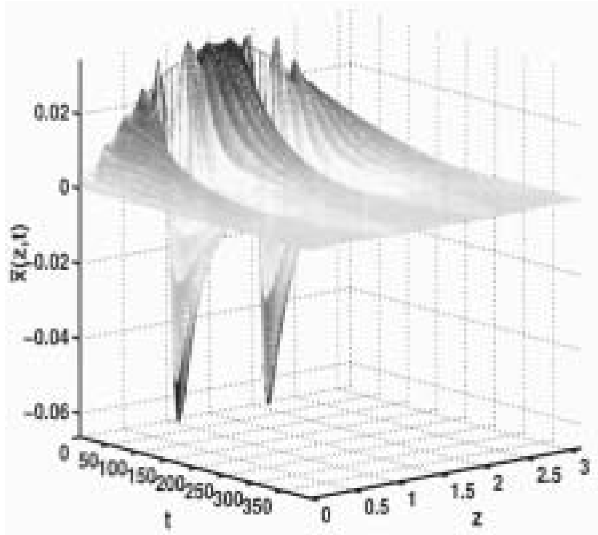

Figure 4. Closed–loop state profile under the MPC formulation Eqs.22–23 without accounting for the fast modal states in the constraints

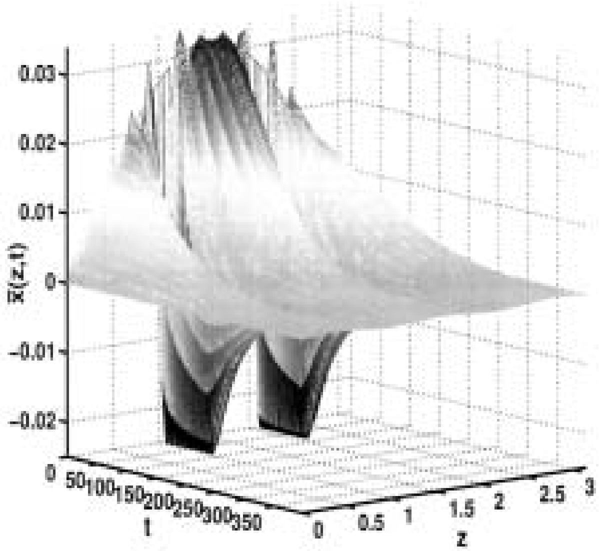

Figure 5. Closed–loop state profile under the MPC formulation Eqs.24–25 with accounting for the fast modal states in the state constraints

invoke the following MPC formulation with the performance functional and constraints given by,

$$\min_{u} \sum_{k=0}^{N-1} \{[a_s(k+i)'Qa_s(k+i)+u(k+i)'Ru(k+i) + GAMMA(a_f(i))]+ +a_s(i+N)'\bar{Q}a_s(i+N)\} \quad (24)$$

$$\text{s.t. } a_s(k+1) = A_s a_s(k) + B_s u(k)$$
$$a_f(k+1) = A_f a_f(k) + B_f u(k) \quad k=0,1,2,...,N-1$$
$$u_j^{min} \le u_j(k) \le u_j^{max} \quad j=1,2 \quad (25)$$
$$\chi_g^{min} - C_f a_f(k) \le C_s a_s(k) \le \chi_g^{max} - C_f a_f(k) \quad g=1,2,...,p$$

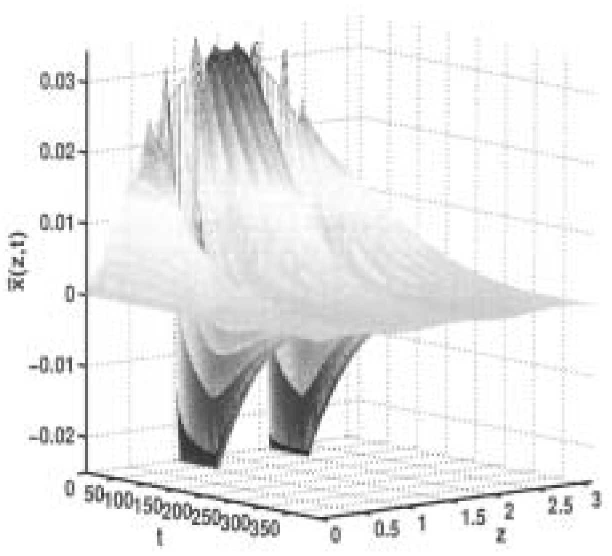

Figure 6. Closed–loop state profile under the MPC formulation Eqs.24–25 with accounting for the fast modal states in the state constraints

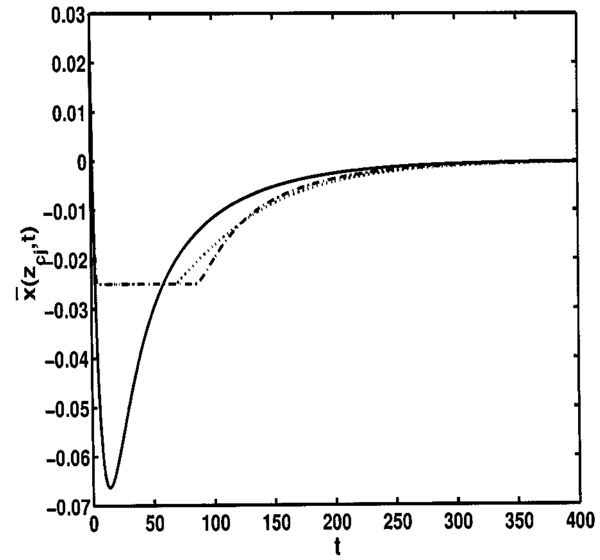

Figure 7. Closed–loop state profile at z_{cj} = $\pi/3$ under the MPC formulation of Eqs. 22–23 without accounting for the evolution of the fast modes (solid), under the MPC formulation Eqs.24–25 with accounting for the fast modal states in the state constraints (dashed–dotted), and under the MPC formulation of Eqs.24–25 with accounting for the fast mode dynamics in the state constraints and in the cost function (dotted)

where $C_f = [\phi_3(z_{cj})\ \phi_4(z_{cj}) \dots \phi_{20}(z_{cj})]$, and the MPC tuning parameters are kept the same as in the previous formulation. In this formulation, the penalty function $\Gamma(a_f)$ on the fast mode dynamics is introduced in the formulation of the constrained optimization problem as a standard method of penalizing the evolution of the fast modes in the optimization functional complemented with their evolution being reflected as a time dependent correction of the constraints of the slow subsystem. The utilization of the MPC formulation, Egs. 24–25, which

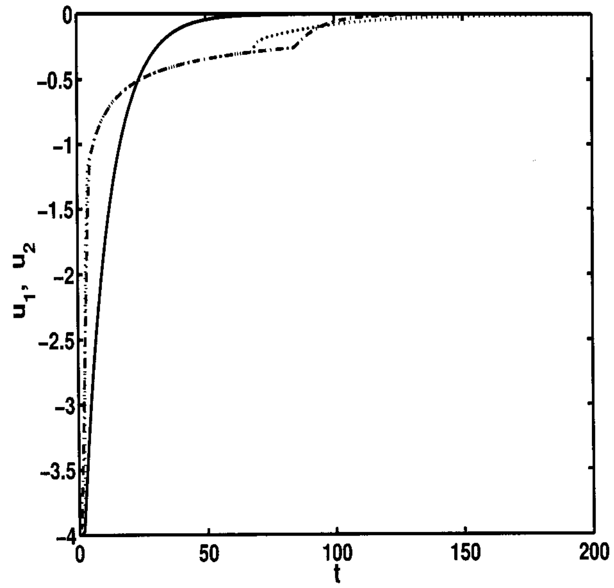

Figure 8. Manipulated input profile for the control actuators applied at z_{c1} = $\pi/3$ and at z_{c2} = $2\pi/3$ under the MPC formulation of Eqs.22–23 (solid), under the MPC formulation Eqs.24–25 (dashed–dotted), and under the MPC formulation of Eqs.24–25 with $\Gamma(x_f)$ (dotted).

accounts for the evolution of the fast modes in the countraints, is demonstrated in Figs.7 and 8 (dashed–dotted lines), as the predictive controller successfully stabilizes the state profile at the zero steady – state and satisfies the full PDE state constraint requirement.

The evolution of the fast modes is represented in the finite horizon constrained optimization problem as a correction term in the constraints on the states of a slow subsystem. In addition, this evolution can be penalized in an appropriate way by way of a penalty function $\Gamma(x_f)$, where penalties can be defined as penalties on the input induced evolution or initial condition induced evolution of the fast modes, at a particular point in the spatial domain (i.e., z_{cj}). In particular and for the sake of demonstration, we consider the case of Eq.13 where matrix $H = I\omega$, $\omega = 100$, so that when Eq.14 is incorporated in Eq.13, it renders the following form expressed as,

$$\Gamma(a_f(i)) = u(i)'Hu(i) + u(i)'Ya_f(0) + a_f(0)'\mathcal{G}a_f(0) \quad i = 1,2,\dots, N-1 \tag{26}$$

where H and G are weighted contributions of the input induced dynamics and initial conditions of the fast modes, and Y is the term that accounts for the mixed contribution of these two dynamics in the performance functional. By introducing this form of a penalty function which accounts for the dynamics of the fast modes along the horizon, we account for the quadratic measure of penalties with respect to the input effort and for the contribution of the initial conditions. Fig.6 and Figs.7–8 (dashed lines) show, that the formulation which accounts for penalties on the fast modes dynamics, slightly improves by the faster stabilization over the one that does not account for the fast modes.

Remark 3: Another type of measure of the penalties of the fast modal dynamics due to the input can be given by the l_∞ norm, which is given as a worst case peaking induced by the input among all points where constraints are required to be enforced. In this case, $\Gamma(a_f(i)) = \|C_f A_f^{i-1} B_F\|_\infty u(i)$, which is added in the optimization functional Eq.24.

To summarize, the comparison between different MPC formulations is used to underline an important fact that the fast states are central to the predictive controller's ability to enforce the state constraints in a closed–loop PDE and must, therefore, be accounted for in the predictive controller design. Along this line, it was demonstrated within the framework of the MPC, that accounting for the fast mode dynamics is accomplished by means of state constraints and by penalizing the undesired fast mode dynamics.

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Appendix 1.

Parabolic infinite dimensional systems: For a precise characterization of the class of PDEs considered in this work, we formulate the PDE of Eq.1 as an infinite dimensional system in Hilbert space $H([0,\pi], IR)$, with H being the space of measurable functions defined on $[0,\pi]$, with the inner product and norm:

$$(\omega_1,\omega_2) = \int_0^\pi (\omega_1(z), \omega_2(z))_{IR_n} dz, \ \|\omega_1\|_2 = (\omega_1,\omega_1)^{\frac{1}{2}} \quad \text{(a)}$$

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

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

the operator A in $H([0,\pi]; IR)$ as:

$$Ax = b\frac{\partial^2 \bar{x}}{\partial z^2} + \alpha\bar{x},$$

$$x \in D(A) = \{x \in H([0,\pi];IR^n) : \bar{x}(0,t) = 0,\ \bar{x}(\pi,t) + 0\} \quad \text{(c)}$$

and the input operator as:

$$Bu = \sum_{i=1}^{m} b_i u_i \quad \text{(d)}$$

the system of equations Eqs.1–3 takes the form:

$$\dot{x} = Ax + Bu,\ x(0) = x_0 \quad \text{(e)}$$

where $x_0 = x_0(z)$. For the operator A, eigenvalue is defined as:

$$A\phi_j = \lambda_j\phi_j,\ j = 1,\ldots,\infty \quad \text{(f)}$$

where λ_j denotes eigenvalue and ϕ_j denotes the eigenfunction. The eigenvalue problem takes the form

$$b\frac{\partial^2\phi_j}{\partial z^2} + \alpha\phi = \lambda_j\phi_j \quad \text{(g)}$$

subject to

$$\phi_j(0) = \phi_j(\pi) = 0 \quad \text{(h)}$$

where b>0. A direct computation of the solution of the above eigenvalue problem yields

$$\lambda_j = \alpha - bj^2,\ \phi_j(z) = \sqrt{\frac{2}{\pi}}\sin(j\,z),\ j = 1,\ldots,\infty \quad \text{(i)}$$

The spectrum of A, $\sigma(A)$, is defined as the set of all eigenvalues of A, i.e. $\sigma(A)=\{\lambda_1,\lambda_2,\ldots\}$. From the expression for the eigenvalues, it is clear that all the eigenvalues of A are real, and that, for a given α and b, only a finite number of eirgenvalues (i.e. λ_j and λ_{j+1} increases as j increases). Furthermore, $\sigma(A)$ can be partitioned as $\sigma(A)=\sigma_1(A)\cup\sigma_2(A)$, where $\sigma_1(A)=\{\lambda_1,\ldots,\lambda_m\}$ contains the first m (with m finite) "slow" (possibly unstable) eigenvalues and $\sigma_2(A)=\{\lambda_{m+1},\lambda_{m+2},\ldots,\}$ contains the remaining "fast" stable eigenvalues. This implies that the dominant dynamics of the PDE can be described by a finite–dimensional system, and motivates the use of modal decomposition to derive a finite–dimensional system that captures the dominant (slow) dynamics of the PDE.

Appendix 2.

Modal decomposition: We apply Galerkin's method to the system of Eq. (e) to derive an approximate finite–dimensional system. Let H_s, H_f be modal subspaces of A, defined as H_s=span $\{\phi_1,\phi_2,...,\phi_m\}$ and H_f = span$\{\phi_{m+1},\phi_{m+2},...,\}$ (the existence of H_s, H_f follows from the properties of A and ϕ_j are eigenfunctions of A). Defining the orthogonal projection operators P_s and P_f such that $x_s=P_sx$, $x_f=P_fx$, the state x of the system of Eq.(e) can be decomposed as:

$$x = x_s + x_f = P_sx + P_fx \qquad ($$

Applying P_s and P_f to the system of Eq.(e) and using the above decomposition for x, the system of Eq.(e) can be equivalently written in the following form:

$$\frac{dx_s}{dt} = A_sx_s + B_su$$

$$\frac{\partial x_f}{\partial t} = A_fx_f + B_fu \qquad ($$

$$y_m = Sx_s + Sx_f,$$

$$x_s(0) = P_sx(0) = P_sx_0,\ x_f(0) = P_fx(0) = P_fx_0$$

where $A_s=P_sA$, $B_s=P_sB$, $A_f=P_fA$, $B_f=P_fB$ and the notation $\frac{\partial x_f}{\partial t}$ is used to denote that the state x_f belongs to an infinite–dimensional space. In the above system, A_s is a diagonal matrix of dimension m x m of the form A_s = diag$\{\lambda_j\}$ (λ_j are eigenvalues of A_s) and A_f is an unbounded differential operator which is exponentially stable (following from the fact that $\lambda_{m+1}<0$ and the selection of H_s, H_f). Neglecting the fast and stable infinite–dimensional x_f–subsystem in the system of Eq.(k), the following m–dimensional slow system is obtained:

$$\frac{d\bar{x}_s}{dt} = A_s\bar{x}_s + B_su \qquad ($$

$$\bar{y}_m = S\bar{x}_s$$

where the bar symbol in $\bar{x}_s$ and $\bar{y}_m$ denotes that these variables are associated with a finitedimensional system.

IZVOD

MODEL PREDSKAZUJUĆE KONTROLE PROCESA DIFUZIJE I HEMIJSKE REAKCIJE

(Naučni rad)

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Parabolične parcijalne diferencijalne jednačine prirodno se pojavljuju kao adekvatno matematičko opisivanje široke klase sistema sa parametrima distribuiranim u prostoru. To su najčešće primeri procesa u kojima difuzija i hemijska reakcija definišu brzinu, gde međusoban odnos između otpora za difuziju i otpora hemijske reakcije uvodi kompleksnost u matematički opis procesa neophodan za potrebe indentifikacije parametara modela i kontrole procesa. U ovom radu se definiše model predskazujuće kontrole (model predictive control - MPK) paraboličnih parcijalnih diferencijalnih jednačina sa odgovarajućim ograničenjima koja definišu pogonske sile i dozvoljena stanja sistema. Model predskazujuće kontrole je jedan od najpopularnijih upravljačkih sistema koji se koristi u hemijskom inženjerstvu, pre svega zbog mogućnosti da se u proračun uključi ograničena vrednost pojedinačnih otpora. Ovi otpori moraju biti uključeni u proračun, s obzirom da pogonske sile (pokretači) ne mogu imati beskonačne vrednosti (na primer pumpa i ventil ne mogu da omoguće beskonačan protok fluida već je on specifikacijom ovih uređaja ograničen) u odnosu na druge zahteve i specikacije procesa. U generisanju predskazujućeg regulatora, koji uzima u obzir granične vrednosti otpora (pokretača), na početku je korišćen Galerkinov metod pomoću koga je, na zadovoljavujući način, parcijalna diferencijalna jednačina paraboličnog tipa transformisana u sistem običnih linearnih diferencijalnih jednačina. Na taj način je definisano početno dozvoljeno stanje sistema. Modifikovana sinteza modela predskazujućeg regulatora koristi određenu formu pomoću koje mogu da budu zadovoljeni zahtevani uslovi dozvoljenog stanja sistema, ali kao novinu, poseduje i penalizovan član koji je sastavni deo optimizacione funkcije modela. Model predskazujuće kontrole (regulatora) uspešno je primenjen za kontrolu linearne parabolične diferencijalne jednačine koja opisuje proces difuzije praćen istovremenom hemijskom reakcijom i uspešno definiše kontrolu i regulaciju temperature oko nestabilnog stacionarnog stanja uz zadovoljenje granične vrednosti pogonske sile za prenos toplote tj. razlike temperature. Sistem kontrole, pri tome, zadovoljava pri regulaciji i stabilizaciji procesa odgovarajuće granične vrednosti pogonske sile.

Ključne reči: Kontrola, Predskazujuća kontrola, Difuzija praćena hemijskom reakcijom, Diferencijalne jednačine, Parcijalne diferencijalne jednačine, Granični i početni uslovi, Galerkinova metoda.