Linear Model Predictive Control for Transport-Reaction Processes

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The article deals with systematic development of linear model predictive control algorithms for linear transport-reaction models emerging from chemical engineering practice. The finite-horizon constrained optimal control problems are addressed for the systems varying from the convection dominated models described by hyperbolic partial differential equations (PDEs) to the diffusion models described by parabolic PDEs. The novelty of the design procedure lies in the fact that spatial discretization and/or any other type of spatial approximation of the process model plant is not considered and the system is completely captured with the proposed Cayley-Tustin transformation, which maps a plant model from a continuous to a discrete state space setting. The issues of optimality and constrained stabilization are addressed within the controller design setting leading to the finite constrained quadratic regulator problem, which is easily realized and is no more computationally intensive than the existing algorithms. The methodology is demonstrated for examples of hyperbolic/parabolic PDEs. © 2016 American Institute of Chemical Engineers *AIChE J*, 00: 000–000, 2016
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Introduction

Modelling of a transport process is the most important issue in the process analysis and control design of transport processes. It is currently addressed by phenomenological modelling arising from first-principles, experimental studies and/or with the help of the system identification theory. In many industries including chemical, petrochemical, and pharmaceutical plants, model-based control has been very successful. In majority of them, the underlying plant model is low dimensional and linear. In general, mathematical models of many industrial relevant transport processes are obtained from conservation laws, such as mass, momentum and/or energy, and take forms represented by nonlinear partial differential equations (PDEs). The salient feature of these models is temporal and spatial dependence that captures the change in shape and material properties, and can be associated with well-known physical phenomena of the phase change, generation or/and consumption of chemical species by chemical reaction mechanisms, heat and mass transfer phenomena.

Chemical process control of lumped parameter systems is a well-established and documented field of the process control. One of the most prominent achievements in the broad area of process control is development of model predictive control for lumped parameter systems.[1–6] This refers to a class of control algorithms which compute a control variable by utilizing a plant process model to optimize a linear or quadratic open-loop performance objective subject to constraints over a future time horizon. The computed control variable profile over the horizon is utilized by applying only the first move and this process is repeated at each time interval in a repetitive manner. In the case of linear models,[3] linear predictive control utilizes a linear state space or transfer function models obtained by the first principles, or obtained by the pulse and/or step response of the controlled plant. The great feature of linear model predictive control is that constrained and multivariable processes can be addressed with emphasis on a robust algorithm realization that can be implemented on-line.

Along the line of developed control areas, the control of linear distributed parameter systems is a mature control field.[7–11] The intrinsic feature of distributed parameter systems is that the models take the form in an infinite dimensional space setting which leads into infinite dimensional controller designs that are not implementable and realizable in practice. In other words, control designers are forced to apply some type of approximations to arrive at some finite dimensional model setting that can be consequently explored within a finite dimensional control design setting. Along this line of work, there are several contributions, for example, the seminal work of Harmon Ray[7] laid foundation for spectral treatment for a class of distributed parameter systems, Ray and Seinfeld explored the design of nonlinear distributed state estimators using stochastic methods.[12] Other notable works addressed the issue of identification and multivarable predictive control applied to distributed parameter systems.[13,14] More recently, Ng and Dubljevic considered the time-varying optimal control problem[15] and boundary control formulation[16] for the crystal growth model regulation with time-varying domain characteristic represented by the PDE as an abstract evolution equation on an infinite-dimensional function space with a nonautonomous parabolic

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operator which generates a two-parameter semigroup. Despite the aforementioned developments and a myriad of work on unconstrained stabilization, the issue of a low order constrained optimal/suboptimal controller design remained elusive.

In the last decade, there were several attempts to address control of distributed parameter systems within an input and/or state constrained optimal control setting. In the case of transport systems modelled by the first order hyperbolic systems, there were several works on dynamical analysis and control of hyperbolic PDEs systems, and in particular, the work of Aksikas et al. on linear quadratic control application to a fixed-bed reactor[17] and optimal linear quadratic feedback controller design to hyperbolic distributed parameter systems.[18] Other contributions considered model predictive control applied to hyperbolic systems.[19,20] In the same vein, the optimal and model predictive control realizations are extended to Riesz spectral systems (parabolic, and higher order dissipative PDEs) with a separable eigenspectrum of the underlying dissipative spectral operator with successful realization of algorithms that account for the input and PDE state constraints.[21–25] There are also other extensions in the area of nonlinear model predictive control[26] in which a combination of on-line model reduction and successive linearizations is applied. In all aforementioned control design realizations, some type of appropriate approximation is applied to a continuous model to arrive to a discrete model, which is used for the controller design. It will be clear in subsequent sections, that one can treat the linear distributed parameter system intact and design a controller without any model approximation.

In this article, we provide development of an optimal constrained finite dimensional controller for linear transport-reaction systems with input and PDE state/output constraints which capture majority of linear transport-reaction chemical process systems of interest. The prominent feature of the proposed controller design is that no spatial discretization is required. The linear transport-reaction system is completely captured with the proposed transformations from a continuous to a discrete state space setting without consideration of spatial discretization and/or any other type of spatial approximation of the process model plant. The Cayley-Tustin time discretization transformation is applied to the parabolic PDE system and hyperbolic PDE system to preserve the infinite-dimensional nature of the distributed parameter system.[27] Along the line of Cayley-Tustin transformation, the time discretization lies in the fact that conservative characteristics of the system are preserved.[28–30] The issues arising from analytic transformation of continuous to discrete distributed parameter setting are addressed by providing guidance for appropriate choice of discretization parameters. An important resolvent operator for discretization realization of parabolic and hyperbolic PDE system is obtained. The underlying analytic form of a discrete model is utilized in the design of the model predictive controller which addresses the input and PDE state/output constraints satisfaction and stabilization by finite dimensional convex quadratic problem realization. The representative examples of the novel algorithm design applied to hyperbolic and parabolic transport-reaction systems are discussed from the stability and optimality point of view.

The article is organized as follows. In "Time Discretization for Linear PDE" section, the Cayley-Tustin time discretization for distributed parameter systems is introduced. Further, the discrete-time model representations for the hyperbolic and parabolic PDE system are provided. In "Model Predictive Control for Linear PDE" section, the model predictive controller is designed and the issues related to stability, input and state constraints satisfaction are addressed. In "Summary" section, we demonstrate the features of the model predictive control algorithm built in the previous section through the simulation studies.

Time Discretization for Linear PDE

The linear infinite-dimensional system is described by the following state space system:

$$\begin{aligned}\dot{z}(\zeta,t)&=Az(\zeta,t)+Bu(t),\ z(\zeta,0)=z_0\\ y(t)&=Cz(\zeta,t)+Du(t)\end{aligned}\tag{1}$$

where the following assumptions hold: the state $z(\zeta,t)\in H$, where H is a real Hilbert space endowed with the inner product $<\cdot,\cdot>$; the input $u(t)\in U$ and the output $y(t)\in Y$, where U and Y are real Hilbert spaces; the operator $A:D(A)\subset H\rightarrow H$ is a generator of a C_0-semigroup on H and has a Yoshida extension operator A_{-1} (to accommodate for boundary or point actuation)[31]; B, C and D are linear operators associated with the actuation and output measurement or direct feed forward element, i.e., $B\in L(U,H)$, $C\in L(H,Y)$ and $D\in L(U,Y)$. In particular, the operator A is a linear spatial operator associated with the hyperbolic or parabolic transport reaction system.

Taking a type of Crank-Nicolson time discretization scheme and given a time discretization parameter $h>0$, in the system engineering theory known as Tustin time discretization is given by[32]:

$$\begin{aligned}\frac{z(jh)-z((j-1)h)}{h}&\approx A\frac{z(jh)+z((j-1)h)}{2}+Bu(jh),\ z(0)=z_0\\ y(jh)&\approx C\frac{z(jh)+z((j-1)h)}{2}+Du(jh)\end{aligned}\tag{2}$$

Let $u_j^h/\sqrt{h}$ be the approximation of $u(jh)$, the convergence of $y_j^h/\sqrt{h}$ to $y(jh)$ as $h\rightarrow 0$ under rather general assumptions, the above set of equations yields the discrete time dynamics:

$$\begin{aligned}\frac{z_j^h-z_{j-1}^h}{h}&=A\frac{z_j^h+z_{j-1}^h}{2}+B\frac{u_j^h}{\sqrt{h}},\ z_0^h=z_0\\ \frac{y_j^h}{\sqrt{h}}&=C\frac{z_j^h+z_{j-1}^h}{2}+D\frac{u_j^h}{\sqrt{h}}\end{aligned}\tag{3}$$

After some basic manipulation, the discrete system takes the following form:

$$\begin{aligned}z(\zeta,k)&=A_dz(\zeta,k-1)+B_du(k),\ z(\zeta,0)=z_0\\ y(k)&=C_dz(\zeta,k-1)+D_du(k)\end{aligned}\tag{4}$$

where $\delta=2/h$, A_d, B_d, C_d, and D_d are discrete time linear system operators, given by

$$\mathcal{S}:=\begin{bmatrix}A_d & B_d\\ C_d & D_d\end{bmatrix}=\begin{bmatrix}[\delta-A]^{-1}[\delta+A] & \sqrt{2\delta}[\delta-A_{-1}]^{-1}B\\ \sqrt{2\delta}C[\delta-A]^{-1} & G(\delta)\end{bmatrix}\tag{5}$$

where $G(\delta)$ denotes the transfer function of the system and is defined as $G(\delta)=C[\delta-A_{-1}]^{-1}B+D$. A continuous system with strictly proper transfer function has physical realization and does not have the feedthrough operator D (e.g., $D=0$).

However, the corresponding discrete representation for the linear transport reaction systems poses the feedthrough operator $D_d = G(\delta)$.[27] This continuous and discrete infinite dimensional system representations discrepancy is nullified in the limit of $h \to 0$, which implies that discrete system given by Eq. 4 becomes a continuous counterpart in the limit given by Eq. 1. Moreover, it is important to notice that if the transfer function of the continuous system Eq. 1 $G(\delta)$ is strictly proper, then the limit of $G(\delta)$ at infinity exists and is 0,[33] which ensures the well posedness of the system. An important notion is that all physically realizable dynamical systems usually do not contain feedthrough operator which represents instantaneous transfer of signal from the input to the output. The mapping between the continuous system (A, B, C, D) to $\mathcal{S}$ discrete infinite dimensional systems is referred as the Cayley-Tustin discretization method. Another important property of this discretization method is that the discretization does not change the nature of the transformed system. Namely, the classical application of the forward in time Euler discretization may potentially transform a stable continuous system into an unstable discrete system, while the backward in time Euler discretization may transform an unstable system into a discrete, stable one.[34] Finally, if the Cayley-Tustin discretization method is applied to a linear conservative continuous time system, then the resulting discrete system is conservative in the discrete time sense. This transformation preserves the energy equality among the continuous and the discrete model, in other words, it is simplectic or Hamiltonian preserving. The Cayley-Tustin discretization method applied is also a symmetric method, which means that the formula in Eq. 2 is left unaltered after exchanging $z_j \leftrightarrow z_{j-1}$ and $h \leftrightarrow -h$.[35]

Remark 1. *The Cayley-Tustin discretization method maps the generator A of the continuous time system to its cogenerator A_d of the corresponding discrete time system. The operator A_d can be also expressed as $A_d = [\delta - A]^{-1}[\delta + A] = -I + 2\delta[\delta - A]^{-1}$, with I being the identity operator.*

Proof. One can easily show:

$$
\begin{aligned}
A_d(\cdot) &= [\delta - A]^{-1}[\delta + A](\cdot) \\
&= \frac{\delta + A}{\delta - A}(\cdot) \\
&= [-I + \frac{2\delta}{\delta - A}](\cdot) \\
&= [-I + 2\delta[\delta - A]^{-1}](\cdot)
\end{aligned}
\tag{6}
$$

In addition to the transformation of a distributed parameter system from continuous to discrete representation, important technical difficulties associated with point and/or boundary actuation and observation in the continuous system representation are remediated with construction of bounded operators associated with (A_d, B_d, C_d, D_d). The Cayley-Tustin transform maps the unbounded operators A, B, and C of the continuous time system into the bounded operators in the discrete-time counterpart, which brings technical advantages, since the generic properties, such as stability, controllability and observability are the same for both representations. In addition, one can extend the formalism of the above section to the analysis of parametric variations on the solution of Eq. 1. This indeed goes well with the notions of dynamic simulators, so called" time-steppers" in[36–38] used to perform fixed-point and path following computations. ■

Linear hyperbolic scalar system

In this section, we are interested in the construction of a discrete model for the convection dominated system, such as the plug flow reactor model.[7] In general, one can apply a spatial discretization and/or use method of characteristic to obtain an approximate linear model suitable for the controller design. However, here we consider the Cayley-Tustin approach by applying a transformation which completely captures the nature of linear infinite-dimensional systems dynamics and translates a first order hyperbolic PDE from a continuous to a discrete state space setting.

Let us consider the model of transport-reaction system given by Eq. 1, which is the linear infinite-dimensional system model on the Hilbert space $L_2(0,1)$, with the spatial linear operator $A = -v\frac{\partial}{\partial \zeta} + \psi(\zeta)$ defined on its domain $D(A) = \{z \in L_2(0,1) | z \text{ is absolutely continuous } \frac{dz}{d\zeta} \in L_2(0,1), z(0) = 0\}$. The output is taken as the state at the exit of the reactor, that is at $\zeta = L$, and it is obtained by the operator $C(f(\zeta)) = \int_0^L f(\zeta)\,\delta(\zeta - L)d\zeta = f(L)$ and we assume that the continuous model does not contain a feedthrough term, that is $D = 0$. The discretized hyperbolic PDE system is obtained by the Cayley-Tustin transformation presented in the previous section by Eq. 4 where the operators A_d, B_d, C_d, and D_d are calculated by Eq. 5. From Remark 1, one can notice that the realization of the operators in Eq. 5 depends on the resolvent $R(\delta, A)$ of the operator A.

The resolvent operator for the scalar hyperbolic system can be obtained by utilizing the Laplace transform. Finding a Laplace transform is one of essential ingredients of obtaining the Cayley-Tustin transform. Under the zero-input condition, the following hyperbolic PDE system arising from Eq. 1 is considered:

$$\dot{z}(\zeta, t) = A(\zeta) z(\zeta, t), \;\; z(\zeta, 0) = z_0 \tag{7}$$

The operator A arises as a model of tubular reactors with a linearized spatial reaction term (that is $\psi(\zeta)$), which models a large number of convection dominated transport processes.

The resolvent operator $R(s, A) = [sI - A]^{-1}$ of the operator $A(\zeta)$ is obtained by applying the Laplace transform and expressed as follows:

$$
\begin{aligned}
R(s, A) z(\zeta, 0) &= [sI - A]^{-1}(\cdot) \\
&= \left[\int_0^\zeta \frac{1}{v}(\cdot) e^{-\frac{1}{v}\int_0^\eta (\psi(\phi) - sI)d\phi} d\eta\right] e^{\frac{1}{v}\int_0^\zeta (\psi(\phi) - sI)d\phi}
\end{aligned}
\tag{8}
$$

Proof. One can directly obtain the above expression by taking the Laplace transform of Eq. 7, and integrating the expression in space, which is given as $z(\zeta, s) = [sI - A]^{-1} z(\zeta, 0) = R(s, A) z(\zeta, 0)$.

$$\frac{\partial z(\zeta, s)}{\partial \zeta} = \frac{1}{v}(\psi(\zeta) - sI) z(\zeta, s) + \frac{1}{v} z(\zeta, 0) \tag{9}$$

By solving the above ODE, one obtains:

$$
\begin{aligned}
z(\zeta, s) &= z(0, s) e^{\frac{1}{v}\int_0^\zeta (\psi - sI)d\phi} \\
&+ \left[\int_0^\zeta \frac{1}{v} z(\eta, 0) e^{-\frac{1}{v}\int_0^\eta (\psi - sI)d\phi} d\eta\right] e^{\frac{1}{v}\int_0^\zeta (\psi - sI)d\phi}
\end{aligned}
\tag{10}
$$

With the boundary condition $z(0, s) = 0$, the resolvent operator of the operator A applied on the state $z(\zeta, 0)$ can be expressed as:

$$
\begin{aligned}
R(s, A) z(\zeta, 0) &= [sI - A]^{-1} z(\zeta, 0) \\
&= \left[\int_0^\zeta \frac{1}{v} z(\eta, 0) e^{-\frac{1}{v}\int_0^\eta (\psi - sI)d\phi} d\eta\right] e^{\frac{1}{v}\int_0^\zeta (\psi - sI)d\phi}
\end{aligned}
\tag{11}
$$

With the system resolvent operator described in the previous section, one can directly obtain the discrete time operators in

Eq. 4. The convenient form to express the operator A_d is in the following form:

$$\begin{aligned} A_d(\cdot) &= [\delta - A]^{-1}[\delta + A](\cdot) \\ &= -(\cdot) + 2\delta\left[\int_0^{\zeta} \frac{1}{v}(\cdot) e^{-\frac{1}{v}\int_0^{\eta}(\psi-\delta)d\phi} d\eta\right] e^{\frac{1}{v}\int_0^{\zeta}(\psi-\delta)d\phi} \end{aligned} \tag{12}$$

The details of derivation for the hyperbolic discrete operator A_d are given in Appendix A. In the above derivation, one can extend the class of systems considered with having velocity as spatial function $v(\zeta)$, and accordingly all above expressions can be easily rewritten to account for it.

Similarly, one can directly obtain the expression for the discrete operator B_d. The operator B in a continuous system can represent point or boundary actuation, or it can represent in-domain actuation. Hence, for $B(\zeta)$ describing an in-domain operator $B(\zeta)$, one can obtain the expression of B_d in the following form:

$$\begin{aligned} B_d &= \sqrt{2\delta}[\delta - A]^{-1}B(\zeta) \\ &= \sqrt{2\delta}\left[\int_0^{\zeta} \frac{1}{v}B(\eta) e^{-\frac{1}{v}\int_0^{\eta}(\psi-\delta)d\phi} d\eta\right] e^{\frac{1}{v}\int_0^{\zeta}(\psi-\delta)d\phi} \end{aligned} \tag{13}$$

In the case of a point or boundary realized actuation, the input operator B is given as $B(\zeta)=\delta(\zeta-\zeta_0)$, with ζ_0 being a point position where the actuation is applied. Therefore, one obtains the expression of B_d in the following form:

$$B_d = \begin{cases} 0, & 0 \le \zeta < \zeta_0 \\ \dfrac{\sqrt{2\delta}}{v}, & \zeta_0 \le \zeta \le L \end{cases}$$

For example, for boundary actuation at $\zeta_0=0$, one obtains $B_d=\frac{\sqrt{2\delta}}{v} e^{\frac{1}{v}\int_0^{\zeta}(\psi-\delta)d\phi}$. For boundary actuation at $\zeta_0=L$, one obtains $B_d=\frac{\sqrt{2\delta}}{v}\delta(\zeta-L)$.

Similarly, one can directly obtain the expression of discrete operators C_d and D_d. In particular, C can be point and/or boundary observation, or the output can be considered in some region. When C is a boundary operator at $\zeta=L$, the operator C_d is obtained as follows:

$$\begin{aligned} C_d(\cdot) &= \sqrt{2\delta}C[\delta - A]^{-1}(\cdot) \\ &= \sqrt{2\delta}\left[\int_0^{L} \frac{1}{v}(\cdot) e^{-\frac{1}{v}\int_0^{\eta}(\psi-\delta)d\phi} d\eta\right] e^{\frac{1}{v}\int_0^{L}(\psi-\delta)d\phi} \end{aligned} \tag{14}$$

The operator D_d is a straight forward representation of the transfer function of the system parameterized by the parameter δ.

$$\begin{aligned} D_d &= C[\delta - A_{-1}]^{-1}B + D \\ &= \left[\int_0^{L} \frac{1}{v}B e^{-\frac{1}{v}\int_0^{\eta}(\psi-\delta)d\phi} d\eta\right] e^{\frac{1}{v}\int_0^{L}(\psi-\delta)d\phi} \end{aligned} \tag{15}$$

One can notice that in the discrete state space representation, the operators (A_d, B_d, C_d, D_d) are parameterized by the term δ which contains the discretization time so that one can relate known spatial and temporal discretization numerical techniques and numerical outcomes associated with them with the Cayley-Tustin discrete state space realization. In particular, it is known that for the first order hyperbolic system, temporal and spatial discretization of the simple $\frac{\partial z}{\partial t}+c\frac{\partial z}{\partial \zeta}=0$ transport problem leads to Courant-Friedrichs-Lewy stability conditions. Namely, for many explicit finite difference schemes for hyperbolic systems in one space dimension, the claim is that for numerical stability it is necessary that $|c\frac{h}{\triangle\zeta}| \le 1$. In other words, this condition can be interpreted as $\frac{\triangle\zeta}{h} \ge |c|$ that the numerical speed of propagation must be greater than or equal to the speed of initial data propagation. Hence, if the numerical scheme cannot propagate the initial data at least as fast as the solution of the differential equation, then the solution of the scheme cannot converge to the solution of the partial differential equation. Since the numerical scheme given by Eqs. 4-5 is unconditionally stable, the numerical integration accuracy in Eqs. 12–15 and the choice of δ needs to be selected adequately. In general, one must carefully choose a reasonable value of $\frac{h}{\triangle\zeta}$ to obtain an accurate enough solution, since the accuracy of the solution can be heavily impacted with arbitrary $\frac{h}{\triangle\zeta}$. ■

Remark 2. *In the case of the application of spatial discretization methods and subsequent temporal discretization which is not a Cayley-Tustin, if there is no feed forward operator D, the discretized approximation system will generate realization* $(\tilde{A}_d, \tilde{B}_d, \tilde{C}_d, 0)$, *without a feedthrough term. Contrary to this case, the Cayley-Tustin discretization generates* D_d *term as a direct transfer function parameterized* δ *term.*

Adjoint operator

In the subsequent section, the construction of the model predictive controller requires finding adjoint operators of (A_d, B_d, C_d, D_d), that is $(A_d^*, B_d^*, C_d^*, D_d^*)$. Therefore, the adjoint operator A_d^* of the generator A_d is defined by the equation:

$$<\Phi, Ad^*\Psi^*> \; = \; <Ad\Phi, \Psi^*> \tag{16}$$

where Φ and Ψ^* are arbitrary spatial functions on the domain $L_2(0,1)$.

The expression of the adjoint operator A_d^* of the discrete operator A_d is given in the following form:

$$A_d^*(\cdot) = -(\cdot) + 2\delta\left[\int_{\zeta}^{L} \frac{1}{v}(\cdot) e^{\frac{1}{v}\int_0^{\eta}(\psi-\delta)d\phi} d\eta\right] e^{-\frac{1}{v}\int_0^{\zeta}(\psi-\delta)d\phi} \tag{17}$$

Similarly, one can obtain the expression of the adjoint operator C_d^* of the discrete operator C_d as below:

$$C_d^*(\cdot) = \sqrt{2\delta}\left[\int_0^{L} \frac{1}{v}(\cdot) d\eta\right] e^{-\frac{1}{v}\int_0^{\zeta}(\psi-\delta)d\phi} e^{\frac{1}{v}\int_0^{L}(\psi-\delta)d\phi} \tag{18}$$

The derivations of adjoint operators A_d^* and C_d^* are given in Appendix B. The adjoint operators B_d^* and D_d^* are self-adjoint: $B_d^*=B_d$ and $D_d^*=D_d$.

Linear parabolic system

In this section, we apply the Cayley-Tustin time discretization to the diffusion dominated model of an axial dispersion reactor described by the parabolic PDE with the Dirichlet, Neumann or Robin boundary condition.[7]

Let us consider a diffusion dominated transport-reaction system which leads to the linear infinite-dimensional system model given by Eq. 1 with the operator A defined on Hilbert space $H=L_2(0,1)$. In particular,

$$\begin{aligned} \dot{z}(\zeta,t) &= Az(\zeta,t) + Bu(t), \;\; z(\zeta,0)=z_0 \\ y(t) &= Cz(\zeta,t) + Du(t) \end{aligned} \tag{19}$$

$A(\zeta)=\frac{\partial^2}{\partial\zeta^2}+\psi I$ is the linear operator defined on its domain $D(A)=\{z \in L_2(0,1) | z \text{ is absolutely continuous}, \frac{dz}{d\zeta} \in L_2(0,1), \frac{d^2z}{d\zeta^2} \in L_2(0,1), \psi \text{ is constant}, \;\; \text{Dirichlet boundary conditions}:$

$z(0)=0=z(1)$, Neumann boundary conditions : $\frac{dz(0)}{d\zeta}=0=\frac{dz(1)}{d\zeta}$, Danckwerts boundary conditions: $\frac{dz(0)}{d\zeta}=Pez(0),\ \frac{dz(1)}{d\zeta}=0\}$.

The output is the state of the PDE at a point within the domain, for example at $\zeta=\zeta_0$ and is obtained by the operator $C(f(\zeta))=\int_0^L f(\zeta)\delta(\zeta-\zeta_0)d\zeta=f(\zeta_0)$ and $D=0$.

The discretization of a parabolic PDE system described in Eq. 4 is obtained by the Cayley-Tustin transformation presented in the previous section with the operators A_d, B_d, C_d, and D_d calculated by Eq. 5. To realize discrete system representation for parabolic PDE, let us consider the parabolic PDE system in the following form:

$$\dot{z}(\zeta,t)=A(\zeta)z(\zeta,t) \tag{20}$$

The realization of the discrete operator A_d is constructed by substitution of the s parameter with the δ in the resolvent operator in the expression for A_d in Eq. 5. One needs to address if any constraints are arising as a result of freely choosing any discretization time $\delta=\frac{2}{h}$. In particular, only one constraint is that the discretization time does not coincide with the eigenvalues of the operator A, the $\delta\notin\sigma(A)$, where $\sigma(A)$ is the point spectrum of the spatial operator A.

Therefore, one may easily apply Laplace transform to the parabolic system described in Eq. 20:

$$sz(\zeta,s)-z(\zeta,0)=\frac{\partial^2 z(\zeta,s)}{\partial\zeta^2}+\psi z(\zeta,s) \tag{21}$$

which leads to:

$$\frac{\partial^2 z(\zeta,s)}{\partial\zeta^2}=(sI-\psi)z(\zeta,s)-z(\zeta,0) \tag{22}$$

Further, one can obtain the following system:

$$\frac{\partial}{\partial\zeta}\begin{bmatrix} z(\zeta,s) \\ \frac{\partial z(\zeta,s)}{\partial\zeta}\end{bmatrix}=\begin{bmatrix}0 & 1\\ s-\psi & 0\end{bmatrix}\begin{bmatrix} z(\zeta,s) \\ \frac{\partial z(\zeta,s)}{\partial\zeta}\end{bmatrix}+\begin{bmatrix}0\\ -z(\zeta,0)\end{bmatrix} \tag{23}$$

which leads to $\bar{Z}(\zeta,s)=\begin{bmatrix} z(\zeta,s) \\ \frac{\partial z(\zeta,s)}{\partial\zeta}\end{bmatrix}$, $\bar{A}=\begin{bmatrix}0 & 1\\ s-\psi & 0\end{bmatrix}$ and $\bar{B}=\begin{bmatrix}0\\ -z(\zeta,0)\end{bmatrix}$:

$$\frac{\partial\bar{Z}(\zeta,s)}{\partial\zeta}=\bar{A}\bar{Z}(\zeta,s)+\bar{B} \tag{24}$$

We can obtain the solution of the above ODE:

$$\bar{Z}(\zeta,s)=e^{\bar{A}\zeta}\bar{Z}(0,s)+\int_0^{\zeta}e^{\bar{A}(\zeta-\eta)}\bar{B}d\eta \tag{25}$$

Since $\bar{A}$ is a constant matrix, one can calculate $e^{\bar{A}\bar{t}}$ with the Laplace inverse transform $e^{\bar{A}\bar{t}}=\mathcal{L}^{-1}\{[sI-\bar{A}]^{-1}\}$:

$$e^{\bar{A}\bar{t}}=\begin{bmatrix}\cosh(\sqrt{s-\psi}\bar{t}) & \frac{1}{\sqrt{s-\psi}}\sinh(\sqrt{s-\psi}\bar{t})\\ \sqrt{s-\psi}\sinh(\sqrt{s-\psi}\bar{t}) & \cosh(\sqrt{s-\psi}\bar{t})\end{bmatrix} \tag{26}$$

which leads to the solution of Eq. 25 as:

$$\begin{aligned}\begin{bmatrix} z(\zeta,s) \\ \frac{\partial z(\zeta,s)}{\partial\zeta}\end{bmatrix}&=\begin{bmatrix}\cosh(\sqrt{s-\psi}\zeta) & \frac{1}{\sqrt{s-\psi}}\sinh(\sqrt{s-\psi}\zeta)\\ \sqrt{s-\psi}\sinh(\sqrt{s-\psi}\zeta) & \cosh(\sqrt{s-\psi}\zeta)\end{bmatrix}\begin{bmatrix} z(0,s) \\ \frac{\partial z(0,s)}{\partial\zeta}\end{bmatrix}\\ &+\int_0^{\zeta}\begin{bmatrix}-\frac{1}{\sqrt{s-\psi}}z(\eta,0)\sinh[\sqrt{s-\psi}(\zeta-\eta)]\\ -z(\eta,0)\cosh[\sqrt{s-\psi}(\zeta-\eta)]\end{bmatrix}d\eta\end{aligned} \tag{27}$$

Finally, we obtains:

$$z(\zeta,s)=\cosh(\sqrt{s-\psi}\zeta)z(0,s)+\frac{1}{\sqrt{s-\psi}}\sinh(\sqrt{s-\psi}\zeta)\frac{\partial z(0,s)}{\partial\zeta}-\int_0^{\zeta}\frac{1}{\sqrt{s-\psi}}z(\eta,0)\sinh[\sqrt{s-\psi}(\zeta-\eta)]d\eta \tag{28}$$

The above expression is obtained as a solution to $z(\zeta,s)=[sI-A]^{-1}z(\zeta,0)$, by the application of the Laplace transform to the parabolic system described in Eq. 20 for the case when $s-\psi>0$. However, it can be demonstrated that the similar and well posed expression will be obtained if $s-\psi<0$. Assuming that, $s-\psi<0$, one obtains $\sqrt{s-\psi}=i\sqrt{\psi-s}$, here $i^2=-1$. We can obtain $\sinh(\sqrt{s-\psi}\zeta)=\sinh(i\sqrt{\psi-s}\zeta)=i\sin(\sqrt{\psi-s}\zeta)$ and $\cosh(\sqrt{s-\psi}\zeta)=\cosh(i\sqrt{\psi-s}\zeta)=\cos(\sqrt{\psi-s}\zeta)$. Then, the state becomes:

$$z(\zeta,s)=\cos(\sqrt{\psi-s}\zeta)z(0,s)+\frac{1}{\sqrt{\psi-s}}\sin(\sqrt{\psi-s}\zeta)\frac{\partial z(0,s)}{\partial\zeta}-\int_0^{\zeta}\frac{1}{\sqrt{\psi-s}}z(\eta,0)\sin[\sqrt{\psi-s}(\zeta-\eta)]d\eta \tag{29}$$

In the following section, without loss of generality we consider the case when the following $s-\psi>0$ holds. As expected in the case of parabolic PDEs, different boundary conditions will lead to different expressions for the resolvent of operator A and associated cogenerator A_d.

Dirichlet boundary conditions

When Dirichlet boundary conditions are applied, $z(0,s)=0=z(1,s)$, one can utilize Eq. 27 and 28, and

$\frac{\partial z(0,s)}{\partial \zeta}=\frac{1}{\sinh(\sqrt{s-\psi})}\int_0^1 z(\eta,0)\sinh[\sqrt{s-\psi}(1-\eta)]d\eta$. The resolvent of the operator A is given as:

$$\begin{aligned} &R(s,A)z(\zeta,0)=[sI-A]^{-1}z(\zeta,0)\\ &=\frac{1}{\sqrt{s-\psi}}\frac{\sinh(\sqrt{s-\psi}\zeta)}{\sinh(\sqrt{s-\psi})}\int_0^1 z(\eta,0)\sinh[\sqrt{s-\psi}(1-\eta)]d\eta\\ &\quad-\int_0^\zeta \frac{1}{\sqrt{s-\psi}}z(\eta,0)\sinh[\sqrt{s-\psi}(\zeta-\eta)]d\eta \end{aligned} \tag{30}$$

Neumann boundary conditions

When Neumann boundary conditions are applied, $\frac{dz(0,s)}{d\zeta}=0=\frac{dz(1,s)}{d\zeta}$ and from Eq. 27 and 28, one obtains $z(0,s)=\frac{1}{\sqrt{s-\psi}}\frac{1}{\sinh(\sqrt{s-\psi})}\int_0^1 z(\eta,0)\cosh[\sqrt{s-\psi}(1-\eta)]d\eta$. The resolvent of operator A is:

$$\begin{aligned} &R(s,A)z(\zeta,0)=[sI-A]^{-1}z(\zeta,0)\\ &=\frac{1}{\sqrt{s-\psi}}\frac{\cosh(\sqrt{s-\psi}\zeta)}{\sinh(\sqrt{s-\psi})}\int_0^1 z(\eta,0)\cosh[\sqrt{s-\psi}(1-\eta)]d\eta\\ &\quad-\int_0^\zeta \frac{1}{\sqrt{s-\psi}}z(\eta,0)\sinh[\sqrt{s-\psi}(\zeta-\eta)]d\eta \end{aligned} \tag{31}$$

Danckwerts boundary conditions

Another important set of boundary conditions is arising from the description of an axial dispersion reactor[7]: $z'(0,t)=P_e z(0,t)$, $z'(1,t)=0$, with P_e being a Peclet number. One obtains:

$$\begin{aligned} \frac{\partial z(1,s)}{\partial \zeta}&=\sqrt{s-\psi}\sinh(\sqrt{s-\psi})z(0,s)+\cosh(\sqrt{s-\psi})\frac{\partial z(0,s)}{\partial \zeta}\\ &\quad-\int_0^1 z(\eta,0)\cosh[\sqrt{s-\psi}(1-\eta)]d\eta=0 \end{aligned} \tag{32}$$

so that $z'(0,s)=P_e z(0,s)$, we obtain:

$$\begin{aligned} z(0,s)&=\frac{\int_0^1 z(\eta,0)\cosh[\sqrt{s-\psi}(1-\eta)]d\eta}{\sqrt{s-\psi}\sinh(\sqrt{s-\psi})+P_e\cosh(\sqrt{s-\psi})}\\ z'(0,s)&=\frac{p_e\int_0^1 z(\eta,0)\cosh[\sqrt{s-\psi}(1-\eta)]d\eta}{\sqrt{s-\psi}\sinh(\sqrt{s-\psi})+P_e\cosh(\sqrt{s-\psi})} \end{aligned} \tag{33}$$

Finally, resolvent can be easily defined.

Discrete time operators and its adjoint operators

Dirichlet Boundary Condition. With the system resolvent operator described in Eq. 30, one can directly obtain the discrete time operators A_d, B_d, C_d, and D_d of a parabolic system presented in Eq. 5:

$$\begin{aligned} &A_d(\cdot)=[-I+2\delta[\delta-A]^{-1}](\cdot)\\ &=-(\cdot)+2\delta\Bigg[\frac{1}{\sqrt{\delta-\psi}}\frac{\sinh(\sqrt{\delta-\psi}\zeta)}{\sinh(\sqrt{\delta-\psi})}\int_0^1(\cdot)\sinh[\sqrt{\delta-\psi}(1-\eta)]d\eta\\ &\quad-\int_0^\zeta\frac{1}{\sqrt{\delta-\psi}}(\cdot)\sinh[\sqrt{\delta-\psi}(\zeta-\eta)]d\eta\Bigg] \end{aligned} \tag{34}$$

$$\begin{aligned} &B_d=\sqrt{2\delta}[\delta-A_{-1}]^{-1}B\\ &=\sqrt{2\delta}\Bigg[\frac{1}{\sqrt{\delta-\psi}}\frac{\sinh(\sqrt{\delta-\psi}\zeta)}{\sinh(\sqrt{\delta-\psi})}\int_0^1 B\sinh[\sqrt{\delta-\psi}(1-\eta)]\Bigg]d\eta\\ &\quad-\int_0^\zeta\frac{1}{\sqrt{\delta-\psi}}B\sinh[\sqrt{\delta-\psi}(\zeta-\eta)]d\eta] \end{aligned} \tag{35}$$

$$\begin{aligned} &C_d(\cdot)=\sqrt{2\delta}C[\delta-A]^{-1}(\cdot)\\ &=\sqrt{2\delta}\Bigg[\frac{1}{\sqrt{\delta-\psi}}\frac{\sinh(\sqrt{\delta-\psi}\zeta_0)}{\sinh(\sqrt{\delta-\psi})}\int_0^1(\cdot)\sinh[\sqrt{\delta-\psi}(1-\eta)]\Bigg]d\eta\\ &\quad-\int_0^{\zeta_0}\frac{1}{\sqrt{\delta-\psi}}(\cdot)\sinh[\sqrt{\delta-\psi}(\zeta_0-\eta)]d\eta] \end{aligned} \tag{36}$$

$$\begin{aligned} &D_d=C[\delta-A_{-1}]^{-1}B+D\\ &=\frac{1}{\sqrt{\delta-\psi}}\frac{\sinh(\sqrt{\delta-\psi}\zeta_0)}{\sinh(\sqrt{\delta-\psi})}\int_0^1 B\sinh[\sqrt{\delta-\psi}(1-\eta)]d\eta\\ &\quad-\int_0^{\zeta_0}\frac{1}{\sqrt{\delta-\psi}}B\sinh[\sqrt{\delta-\psi}(\zeta_0-\eta)]d\eta \end{aligned} \tag{37}$$

The expression of an adjoint operator A_d^* of a discrete operator A_d is in the following form:

$$\begin{aligned} A_d^*(\cdot)=-(\cdot)+2\delta\Bigg[&\frac{1}{\sqrt{\delta-\psi}}\frac{\sinh[\sqrt{\delta-\psi}(L-\zeta)]}{\sinh(\sqrt{\delta-\psi})}\\ &\int_0^1(\cdot)\sinh(\sqrt{\delta-\psi}\eta)d\eta\\ &-\int_\zeta^1\frac{1}{\sqrt{\delta-\psi}}(\cdot)\sinh[\sqrt{\delta-\psi}(\eta-\zeta)]d\eta\Bigg] \end{aligned} \tag{38}$$

The derivation for A_d^* is given in Appendix C. The adjoint operator B_d^* is self-adjoint: $B_d^*=B_d$. For other boundary conditions, one can easily find discrete operators and adjoint cogenerators which take the similar form as the one calculated in the case of Dirichlet boundary conditions. The case of Neumann boundary conditions is given in Appendix D.

Model Predictive Control for Linear PDE

The linear discrete-time model dynamics developed in Eq. 4 is utilized in the formulation of the model predictive control for linear transport-reaction systems. The regulator is based on the similar formulation emerging from the finite dimensional systems theory. In particular, there are similarities among constrained optimal controller design formulations for finite and infinite dimensional systems. The important differences in the controller synthesis are associated with the issue how the stable and unstable infinite dimensional systems are treated and this will be discussed in detail in the context of linear transport-reaction model equations. Along the line of similarities, the well-known formulation of the quadratic form optimization functional on the infinite horizon is used for both infinite and finite dimensional systems. That is, minimization of the following open-loop objective functional is given in the form of inner products. Here, at a given sampling time k, the objective function with constraints is given as:

$$
\begin{aligned}
\min_{u^N} \sum_{j=0}^{\infty} &< y(\zeta,k+j|k), Qy(\zeta,k+j|k) > + \\
&< u(k+j+1|k), Ru(k+j+1|k) > \\
s.t.\ z(\zeta,k+j|k) &= A_d z(\zeta,k+j-1|k) + B_d u(k+j|k) \\
y(\zeta,k+j|k) &= C_d z(\zeta,k+j-1|k) + D_d u(k+j|k) \\
u^{\min} &\le u(k+j|k) \le u^{\max} \\
y^{\min} &\le y(\zeta,k+j|k) \le y^{\max}
\end{aligned}
\tag{39}
$$

where Q is a positive semidefinite spatial operator associated with the output (state of PDE) and R is a positive definite spatial operator. The $y(k+j|k)$ and $u(k+j+1|k)$ represent the output and input variables at the future time $k+j$ given the current time k. The vectors Y and U are given as follows:

$$
\begin{aligned}
Y &= [\, y(\zeta,k+1|k) \quad y(\zeta,k+2|k) \quad y(\zeta,k+3|k) \quad \cdots \quad y(\zeta,k+N-1|k) \,]^T \\
U &= [\, u(k+1|k) \quad u(k+2|k) \quad u(k+3|k) \quad \cdots \quad u(k+N-1|k) \,]^T
\end{aligned}
$$

The infinite horizon open-loop objective function in Eq. 39 can be cast as the finite horizon open-loop objective function with an assumption that the input is zero beyond the control horizon, that is $u(k+N|k)=0$, and with inclusion of the terminal penalty term:

$$
\begin{aligned}
\min_{u^N} \ J = \sum_{j=0}^{N-1} &< y(\zeta,k+j|k), Qy(\zeta,k+j|k) > \\
&+ < u(k+j+1|k), Ru(k+j+1|k) > \\
&+ < z(\zeta,k+N-1|k), \bar{Q} z(\zeta,k+N-1|k) >
\end{aligned}
\tag{40}
$$

Without the loss of generality and with the assumption of observability, the output terminal penalty term is replaced with the corresponding state penalty operator term. The issue of how to determine the terminal state penalty term, the operator $\bar{Q}$, depends on the nature of the underlying transport-reaction linear model (that is a parabolic or a hyperbolic PDE system), and whether the system is a stable or unstable one. In general and in similar way as it is done for stable finite dimensional systems, the spatial operator $\bar{Q}$ for the stable PDE model is defined as the infinite sum $\bar{Q} = \sum_{i=0}^{\infty} A_d^{*i} C_d^* Q C_d A_d^i$. Therefore, the operator $\bar{Q}$ can be calculated from the solution of the following operator discrete Lyapunov function:

$$
A_d^* \bar{Q} A_d - \bar{Q} = -C_d^* Q C_d \tag{41}
$$

The straightforward algebraic manipulation of the objective function presented in Eq. 40 results in the following finite dimensional quadratic optimization problem:

$$
\begin{aligned}
\min_{U} \quad J = U^T &< I, H > U + 2U^T < I, Pz(\zeta,k|k) > \\
+ &< z(\zeta,k|k), \bar{Q} z(\zeta,k|k) > + < y(\zeta,k|k), Qy(\zeta,k|k) >
\end{aligned}
\tag{42}
$$

where H and P are computed as below:

$$
H = \begin{bmatrix}
D_d^* Q D_d + B_d^* \bar{Q} B_d + R & B_d^* C_d^* Q D_d + B_d^* A_d^* \bar{Q} B_d & \cdots & B_d^* A_d^{*N-3} C_d^* Q D_d + B_d^* A_d^{*N-2} \bar{Q} B_d \\
D_d^* Q C_d B_d + B_d^* \bar{Q} A_d B_d & D_d^* Q D_d + B_d^* \bar{Q} B_d + R & \cdots & B_d^* A_d^{*N-4} C_d^* Q D_d + B_d^* A_d^{*N-3} \bar{Q} B_d \\
\vdots & \vdots & \ddots & \vdots \\
D_d^* Q C_d A_d^{N-3} B_d + B_d^* \bar{Q} A_d^{N-2} B_d & D_d^* Q C_d A_d^{N-4} B_d + B_d^* \bar{Q} A_d^{N-3} B_d & \cdots & D_d^* Q D_d + B_d^* \bar{Q} B_d + R
\end{bmatrix}
$$

$$
P = \begin{bmatrix}
D_d^* Q C_d + B_d^* \bar{Q} A_d \\
D_d^* Q C_d A_d + B_d^* \bar{Q} A_d^2 \\
\vdots \\
D_d^* Q C_d A_d^{N-2} + B_d^* \bar{Q} A_d^{N-1}
\end{bmatrix}
$$

The objective function given in Eq. 42 is subjected to the following constraints:

$$
\begin{aligned}
U^{\min} &\le U \le U^{\max} \\
Y^{\min} &\le SU + Tz(\zeta,k|k) \le Y^{\max}
\end{aligned}
\tag{43}
$$

One obtains:

$$
\begin{bmatrix} I \\ -I \\ S \\ -S \end{bmatrix} U \le
\begin{bmatrix} U^{\max} \\ -U^{\min} \\ Y^{\max} - Tz(\zeta,k|k) \\ -Y^{\min} + Tz(\zeta,k|k) \end{bmatrix}
$$

where

$$S=\begin{bmatrix} D_d & 0 & 0 & \cdots & 0 \\ C_dB_d & D_d & 0 & \cdots & 0 \\ C_dA_dB_d & C_dB_d & D_d & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ C_dA_d^{N-3}B_d & C_dA_d^{N-4}B_d & C_dA_d^{N-5}B_d & \cdots & D_d \end{bmatrix}$$

$$T=\begin{bmatrix} C_d \\ C_dA_d \\ C_dA_d^2 \\ \vdots \\ C_dA_d^{N-2} \end{bmatrix}$$

In the above case, the constraint is at the output which is taken as the state at $\zeta=L$. One can also have the constraint at any point within domain at $\zeta=\zeta_0$. As a result, the matrix S and T will change by using different discrete operators $\overline{C_d}$ and $\overline{D_d}$.

A standard formulation of the quadratic programming problem in Eq. 42 with constraints leads to the finite dimensional quadratic programming problem with linear constraints that can be easily evaluated. This leads to the well-known formulation of the model predictive controller design emerging from the finite dimensional theory, that if the system is optimizable then the system is stabilizable with satisfaction of input and state constraints, which is guaranteed under no disturbance conditions.

Remark 3. *When the regulator is based on the state, the minimization of the following open-loop objective function is considered*:

$$\min_{u^N} \sum_{j=0}^{\infty} <z(\zeta,k+j|k), Qz(\zeta,k+j|k)> + < u(k+j+1|k), Ru(k+j+1|k)> \tag{44}$$

the terminal state penalty operator becomes $\bar{Q}=\sum_{i=0}^{\infty} A_d^{*i} Q A_d^i$ *and can be calculated from the solution of the following discrete Lyapunov function*:

$$A_d^*\bar{Q}A_d-\bar{Q}=-Q \tag{45}$$

The operators H, P, S, and T are given as follows:

$$H=\begin{bmatrix} B_d^*\bar{Q}B_d+R & B_d^*A_d^*\bar{Q}B_d & B_d^*A_d^{*2}\bar{Q}B_d & \cdots & B_d^*A_d^{*N-1}\bar{Q}B_d \\ B_d^*\bar{Q}A_dB_d & B_d^*\bar{Q}B_d+R & B_d^*A_d^*\bar{Q}B_d & \cdots & B_d^*A_d^{*N-2}\bar{Q}B_d \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ B_d^*\bar{Q}A_d^{N-1}B_d & B_d^*\bar{Q}A_d^{N-2}B_d & B_d^*\bar{Q}A_d^{N-3}B_d & \cdots & B_d^*\bar{Q}B_d+R \end{bmatrix}$$

$$P=\begin{bmatrix} B_d^*\bar{Q}A_d \\ B_d^*\bar{Q}A_d^2 \\ \vdots \\ B_d^*\bar{Q}A_d^N \end{bmatrix},\quad S=\begin{bmatrix} B_d & 0 & \cdots & 0 \\ A_dB_d & B_d & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ A_d^{N-1}B_d & A_d^{N-2}B_d & \cdots & B_d \end{bmatrix},\quad T=\begin{bmatrix} A_d \\ A_d^2 \\ \vdots \\ A_d^N \end{bmatrix}$$

Model predictive control for hyperbolic PDE

Discrete Lyapunov Function. The realization of the model predictive controller given in quadratic program Eq. 42 contains the term $\bar{Q}$ which is obtained as solution of Eq. 41 or Eq. 45. The discrete Lyapunov function $V(k)$ of the hyperbolic or parabolic PDE system is defined as below:

$$V(k)= < z(\zeta,k), \bar{Q}z(\zeta,k) > = \int_0^L z^T(\zeta,k)\bar{Q}z(\zeta,k)d\zeta \tag{46}$$

Straightforward algebraic manipulation of the above discrete Lyapunov function between instances $V(k)$ and $V(k+1)$ results in the following expression of a discrete Lyapunov equation:

$$<z(\zeta,k), [A_d^*\bar{Q}A_d-\bar{Q}]z(\zeta,k)> = - < z(\zeta,k), C_d^*QC_dz(\zeta,k)> \tag{47}$$

It is known that A_d is the infinitesimal cogenerator of the stable A operator that generates a stable C_0-semigroup $\mathcal{T}(t)$ on the Hilbert space H. Therefore, the corresponding power generator in a discrete setting T is power stable if and only if there exists a positive operator $\bar{Q} \in L_2(0,1)$ such that the expression in Eq. 47 for Lyapunov function holds. In other words, the solution $\bar{Q}$ satisfies the following equation:

$$A_d^*\bar{Q}A_d-\bar{Q}=-C_d^*QC_d \tag{48}$$

However, one can notice that the operator $\bar{Q}$ needs to operate on some function which is also true for the operators A_d and C_d and a solution for $\bar{Q}$ in Eq. 48 cannot be directly determined by calculation. The way to calculate the operator $\bar{Q}$ is to link the solution of the discrete and continuous Lyapunov equation for the hyperbolic and parabolic linear transport-reaction PDEs. In particular, it can be demonstrated that the unique solution of the continuous Lyapunov equation is directly related to the discrete one. One can find a unique solution $\bar{Q}$ of the continuous Lyapunov equation:

$$A^*\bar{Q}+\bar{Q}A=-C^*QC \tag{49}$$

and it can be shown that $\bar{Q}$ is also the solution to the discrete Lyapunov equation described in Eq. 48.

One can demonstrate that if the continuous Lyapunov equation $A^*\bar{Q}+\bar{Q}A=-C^*QC$ holds, by simple algebraic manipulation one can obtain:

$$\begin{aligned}A_d^*\bar{Q}A_d-\bar{Q}&=\sqrt{2\delta}[\delta-A]^{-1*}[A^*\bar{Q}+\bar{Q}A]\sqrt{2\delta}[\delta-A]^{-1}\\&=-\sqrt{2\delta}[\delta-A]^{-1*}[C^*QC]\sqrt{2\delta}[\delta-A]^{-1}\\&=-[\sqrt{2\delta}C[\delta-A]^{-1}]^*Q[\sqrt{2\delta}C[\delta-A]^{-1}]\\&=-C_d^*QC_d\end{aligned}$$

Therefore, by multiplying a spatial function $X(\zeta)\in L_2(0,1)$ on both sides of the continuous Lyapunov equation described in Eq. 49 one obtains:

$$A^*\bar{Q}X+\bar{Q}AX=-C^*QCX$$

$$\left[v\frac{\partial\bar{Q}X}{\partial\zeta}+\psi\bar{Q}X\right]+\bar{Q}\left[-v\frac{\partial X}{\partial\zeta}+\psi X\right]=-C^*QCX$$

$$v\bar{Q}\frac{\partial X}{\partial\zeta}+v\frac{\partial\bar{Q}}{\partial\zeta}X+\psi\bar{Q}X-v\bar{Q}\frac{\partial X}{\partial\zeta}+\psi\bar{Q}X=-C^*QCX$$

Finally, one can obtain the solution of the continuous Lyapunov equation by obtaining the analytic solution for the operator $\bar{Q}$ in the case of a hyperbolic PDE in the following equation:

$$\begin{gathered}v\frac{\partial\bar{Q}}{\partial\zeta}X+2\psi\bar{Q}X=-C^*QCX\\ \bar{Q}\in\mathcal{D}(A^*)\end{gathered}\tag{50}$$

In the case when the full state feedback is considered, which implies that the output operator C is a constant, for example $C=1$, then $C^*=C$ which implies that one can remove the arbitrary test function $X(\zeta)$ on both sides in Eq. 50. On the other hand, if C measurement is applied to boundary or point observation, for example at the exit of the reactor in the case of a hyperbolic PDE system, that is $C(f(\zeta))=\int_0^L f(\zeta)\delta(\zeta-L)d\zeta=f(L)$, then C^* is a spatial operator $C^*(f(\zeta))=\int_0^L f(\eta)d\eta\delta(\zeta-L)$, that operates on the arbitrary function $X(\zeta)$.

Remark 4. *In the case of a scalar hyperbolic PDE, it can be shown that the form of a linear hyperbolic PDE given in this work is always stable one, and the issue of calculating the $\bar{Q}$ for an unstable PDE system can arise only in the case of a parabolic PDE.*

Simulation results of model predictive controller design and application to scalar hyperbolic PDE

In simulation, we choose the output of the tubular reactor to represent the output operator, that is $C(f(\zeta))=\int_0^L f(\zeta)\delta(\zeta-L)d\zeta=f(L)$, a uniform state weight function in the Lyapunov function is chosen as $Q(\zeta)=5$, and the arbitrary function $X(\zeta)=1$. By application of the following condition $\bar{Q}\in\mathcal{D}(A^*)$, the integration is obtained by integrating Eq. 50 from $\bar{Q}(\zeta=L)=0$ to $\zeta=0$, see Figure 1. To demonstrate successful application of the model predictive controller, the discretization time $h=0.05$ is chosen, which implies that the $\delta=40$, and $d\zeta=0.01$ is chosen for numerical integration. The model system parameters are chosen as $v=1$, $\psi=0.5$, with constant spatial function $B=2$, $Q=5$ and $R=10$. The initial condition is $z_0=1-\cos(2\pi\zeta)$ and MPC horizon is 15. The constraints for the input and output/state are given as $-0.08\le u(k)\le 0.01$ and $-0.1\le y(k)\le 0.7$.

The controller performance can be evaluated in Figures 3 and 4, and the corresponding control input is given in Figure 2. Figure 3 provides a comparison of outputs $y(k)$ evolution with and without MPC control applied. The state $z(\zeta,k)$ with MPC is shown in Figure 4.

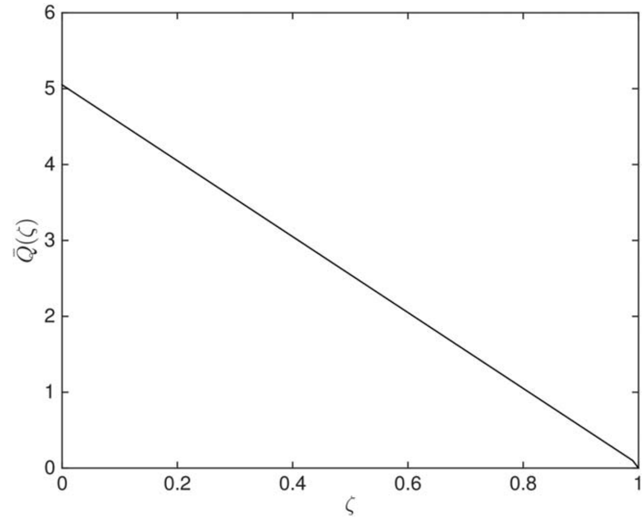

Figure 1. Function $\bar{Q}(\zeta)$ obtained as solution of Eq. 50.

Model predictive control for parabolic PDE

Discrete Lyapunov Function. In the previous section, it has been demonstrated how one can calculate the terminal penalty operator $\bar{Q}$ in the case of a hyperbolic system. However, when it comes to parabolic systems the calculation of $\bar{Q}$ cannot be completed in analytic sense. It can be shown that the solution of a discrete Lyapunov equation $A_d^*\bar{Q}A_d-\bar{Q}=-C_d^*QC_d$ can be obtained by solving a continuous Lyapunov equation $A^*\bar{Q}+\bar{Q}A=-C^*QC$. The continuous Lyapunov equation of parabolic PDE system is consider in the following inner product form[9]:

$$<Az_1,\bar{Q}z_2>+<\bar{Q}z_1,Az_2>=-<Cz_1,QCz_2>\tag{51}$$

where z_1, $z_2\in\mathcal{D}(A)$. Let us take $z_1=\phi_n$ and $z_1=\phi_m$, where ϕ_i represent normalized eigenfunctions of the parabolic linear

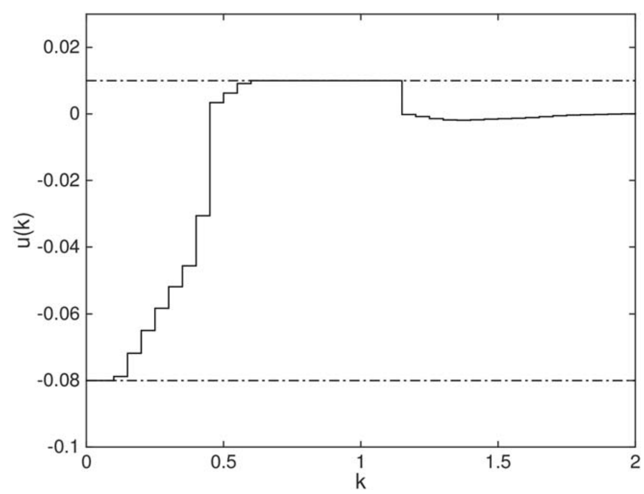

Figure 2. Input profile model predictive control law Eqs. 40–43 constructed on the basis of a discrete time hyperbolic PDE system Eq. 4 with input and output constraints (solid line); input constraints are given by (dash-dot line).

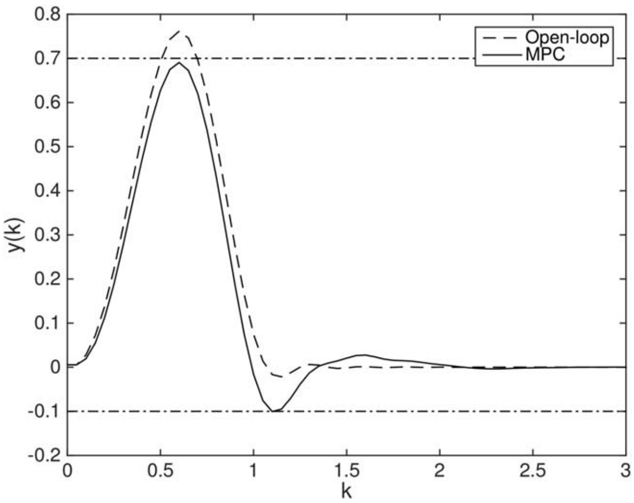

Figure 3. Comparison between the profile of a closed-loop system under the implementation of the model predictive control law Eqs. 40–43 constructed on the discrete time hyperbolic PDE system Eq. 4 with input and output constraints (solid line) and the profile of an open-loop system (dashed line); output constraints (dash-dot line).

operator A. Defining the operator $\bar{Q}_{nm}=<\phi_n,\bar{Q}\phi_m>$, one can obtain:

$$<A\phi_n,\bar{Q}\phi_m>+<\bar{Q}\phi_n,A\phi_m>=-<C\phi_n,QC\phi_m> \tag{52}$$

With $A\phi_n=\lambda_n\phi_n$, the above equation becomes:

$$\lambda_n\bar{Q}_{nm}+\lambda_m\bar{Q}_{nm}=-<C\phi_n,QC\phi_m> \tag{53}$$

then,

$$\bar{Q}_{nm}=-\frac{<C\phi_n,QC\phi_m>}{\lambda_n+\lambda_m} \tag{54}$$

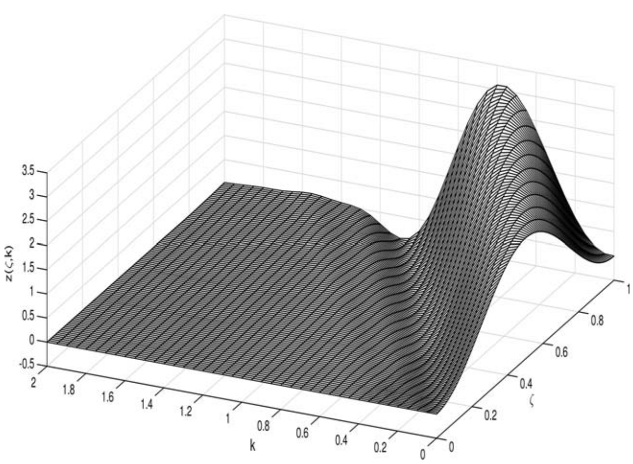

Figure 4. State profile evolution under the applied model predictive control law Eqs. 40–43 constructed on the basis of the discrete time hyperbolic PDE system Eq. 4 with input and output constraints.

Finally, one can obtain the operator $\bar{Q}$ as a solution of continuous Lyapunov equation by calculating the following equation:

$$\begin{aligned}\bar{Q}(\cdot)&=\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\bar{Q}_{nm}<\cdot,\phi_m>\phi_n\\&=\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}-\frac{<C\phi_n,QC\phi_m>}{\lambda_n+\lambda_m}<\cdot,\phi_m>\phi_n\end{aligned} \tag{55}$$

If the operator C is a constant spatial function, then $\bar{Q}_{nm}=-\frac{C^2<\phi_n,Q\phi_m>}{\lambda_n+\lambda_m}$. Since $<\phi_n,Q\phi_m>=\delta_{nm}$, when $n\neq m$, $\bar{Q}_{nm}=0$, thus, $\bar{Q}_{nn}=-\frac{C^2<\phi_n,Q\phi_n>}{2\lambda_n}$, the expression for the operator $\bar{Q}$ simplifies to:

$$\bar{Q}(\cdot)=\sum_{n=0}^{\infty}-\frac{C^2<\phi_n,Q\phi_n>}{2\lambda_n}<\cdot,\phi_n>\phi_n \tag{56}$$

Stability. The definition of a positive definite operator is that if the inner product $<\psi(\zeta),\bar{Q}\psi(\zeta)>$ is nonnegative, the operator $\bar{Q}$ is a positive definite operator. Here, it can be shown that the operator $\bar{Q}$ in Eq. 56 is a positive definite operator. Let us consider:

$$\begin{aligned}<\psi(\zeta),\bar{Q}\psi(\zeta)>&=\int_0^1\psi(\zeta)[\bar{Q}\psi(\zeta)]d\zeta\\&=\int_0^1\psi(\zeta)\left[\sum_{n=0}^{\infty}-\frac{C^2<\phi_n,Q\phi_n>}{2\lambda_n}<\psi(\eta),\phi_n(\eta)>\phi_n(\zeta)\right]d\zeta\\&=\sum_{n=0}^{\infty}-\frac{C^2<\phi_n,Q\phi_n>}{2\lambda_n}<\psi(\eta),\phi_n(\eta)>\left[\int_0^1\psi(\zeta)\phi_n(\zeta)d\zeta\right]\\&=\sum_{n=0}^{\infty}-\frac{C^2<\phi_n,Q\phi_n>}{2\lambda_n}<\psi(\eta),\phi_n(\eta)><\psi(\zeta),\phi_n(\zeta)>\\&=\sum_{n=0}^{\infty}-\frac{C^2<\phi_n,Q\phi_n>}{2\lambda_n}<\psi,\phi_n>^2\end{aligned} \tag{57}$$

Since $Q(\zeta)$ is a nonnegative spatial function, then $<\phi_n,Q\phi_n>=\int_0^1 Q(\zeta)\phi_n^2(\zeta)d\zeta$ is nonnegative. And the eigenvalues of the stable operator A are negative $\lambda_n<0$, thus, the above inner product is nonnegative which implies that the operator $\bar{Q}$ is a positive operator.

If the system is unstable with nonnegative eigenvalues $\lambda_n\geq 0$, $\bar{Q}$ is not a positive definite operator. To address the unstable parabolic PDE, one needs to identify the unstable modes of the continuous linear PDE. The issue to address is that the unstable modes are associated with nonnegative eigenvalues λ_n. Therefore, to guarantee stabilization, one needs to employ the stability constraints in the optimization problem cast as equality constraints. Therefore, if optimization is feasible, the controller will achieve stabilization by cancelling the unstable modes. The corresponding condition is given with the following inner product:

$$<z(\zeta,N),\phi_u>=0 \tag{58}$$

where ϕ_u are the eigenfunctions associated with the nonnegative eigenvalues.

The above equation leads to the following equality constraint expressed as stabilization of unstable modes at the end of the horizon with the feasible input:

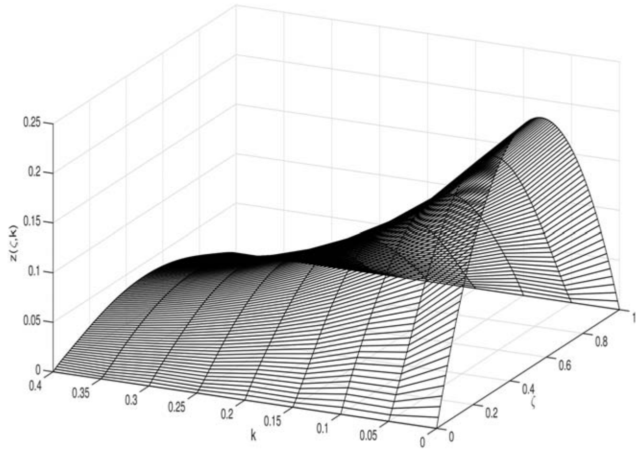

Figure 5. Evolution of the state profile of an open-loop parabolic PDE system Eq. 4 with Dirichlet boundary conditions.

$$\begin{bmatrix} <A_d^{N-1}B_d,\phi_u> & <A_d^{N-2}B_d,\phi_u> & \cdots & <B_d\,,\phi_u> \end{bmatrix} \begin{bmatrix} u(1) \\ u(2) \\ \vdots \\ u(N) \end{bmatrix} = - <A_d^N z(\zeta,0),\phi_u> \tag{59}$$

Equation 59 needs to be integrated in the constrained convex optimization problem given by Eqs. 44 and 45.

Simulation of model predictive controller design and application to scalar parabolic PDE

Dirichlet Boundary Condition. We consider the case of the Dirichlet boundary condition $z(0)=0=z(1)$, and linear operator $A=\frac{\partial^2}{\partial\zeta^2}+\psi$, with ψ being constant. The operator A has eigenvalues $\lambda_n=-n^2\pi^2+\psi$ which determine stability of the system and associated eigenvectors $\phi_n(z)=\sqrt{2}\sin(n\pi z)$, $n\geq 1$.

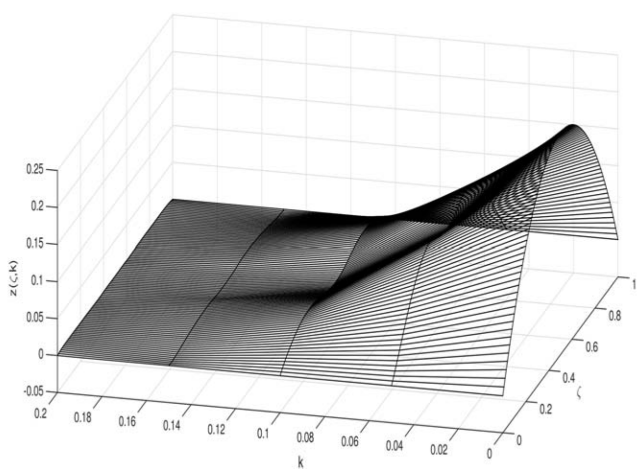

Figure 6. Evolution of the state profile when the model predictive control law Eq. 44 is applied with the Dirichlet boundary condition and input and state constraints.

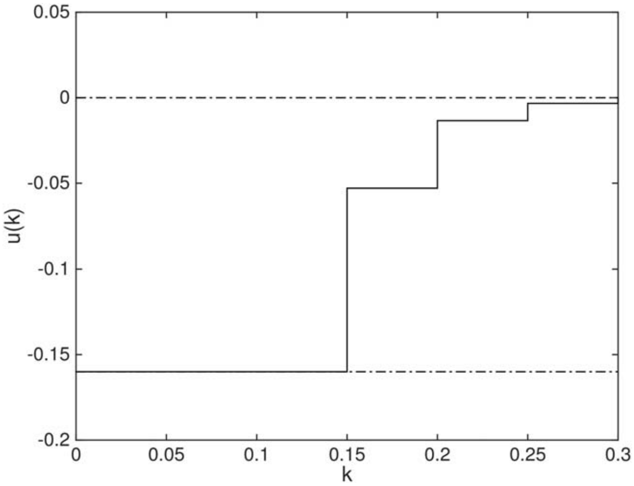

Figure 7. Input profile evolution under the model predictive control law Eq. 44 applied with the Dirichlet boundary condition, input and state constraints. (solid line); input constraints (dash-dot line).

In the case when $\psi<\pi^2$, which implies that the $\lambda<0$, the parabolic system with the Dirichlet boundary condition is stable, see Figure 5. The application of the model predictive controller leads to the faster convergence to the stable steady state with satisfaction of the input and state constraints, see Figures 6–8. In simulation, the system parameters are $\psi=5$, while the actuation distribution function is given as $B=0\,(0<\zeta<0.4\,\&\,0.6<\zeta<1)$ and $B=1\,(0.4<\zeta<0.6)$, $Q=5$ and $R=0.01$. Initial condition is $z_0=-(\zeta-0.5)^2+0.5^2$, and $h=0.05$, with MPC horizon 5. The value of the terminal penalty is calculated by accounting for 5 eigenmodes, that is $n=m=5$. The constraints on the input and the state are given as $-0.16\leq u(k)\leq 0$ and $0\leq z(0.5,k)\leq 0.3$.

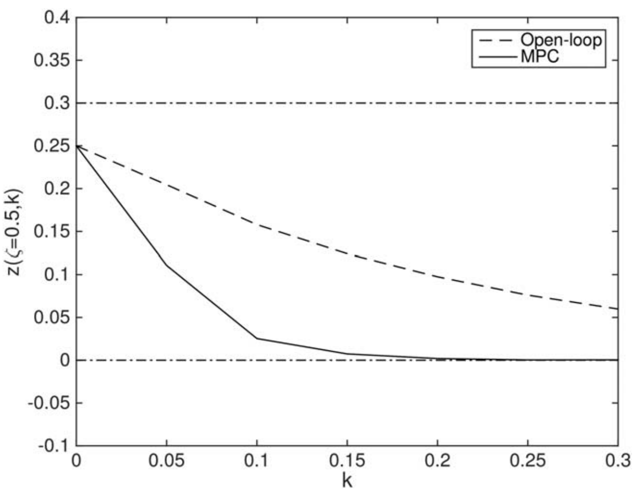

Figure 8. Comparison among profiles of the closed-loop system under the implementation of the model predictive control law Eq. 44 constructed as a discrete time parabolic PDE system in Eq. 4 with the Dirichlet boundary condition and input and state constraints (solid line) and open-loop system profile (dashed line); state constraints (dash-dot line).

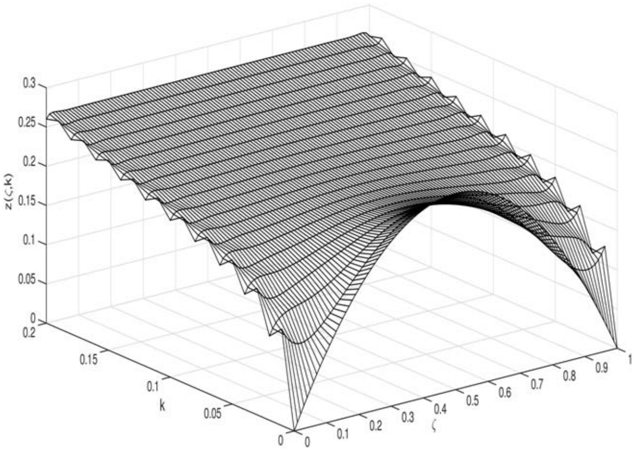

Figure 9. The evolution of state profile of the open-loop parabolic PDE system Eq. 4 with the Neumann boundary condition.

Neumann Boundary Condition. The Neumann boundary condition $\frac{\partial z(0)}{\partial \zeta}=0=\frac{\partial z(1)}{\partial \zeta}$, with the linear operator $A=\frac{\partial^2}{\partial \zeta^2}+\psi$ is considered. The operator A has eigenvalues $\lambda_n=-n^2\pi^2+\psi$, $n \geq 0$ and eigenvectors $\phi_n(z)=\sqrt{2}cos(n\pi z)$, $n \geq 1$, $\phi_0(z)=1$. When $\psi \geq 0$, $\lambda_0 \geq 0$, the parabolic system with Neumann Boundary Condition is unstable, see Figure 9. The application of MPC control law leads to simultaneous stabilization, input and stat/output constraints satisfaction providing that optimization is feasible, see 10-11-12. In simulation studies, the system parameters are $\psi=2$, $B=0\,(0<\zeta<0.4\,\&\,0.6<\zeta<1)$ and $B=1\,(0.4<\zeta<0.6)$, $Q=5$, and $R=0.01$. The initial condition is $z_0=-(\zeta-0.5)^2+0.5^2$, $h=0.01$ and the MPC horizon is 5. The value of the terminal penalty is calculated by accounting for 10 eigenmodes, that is $n=m=10$. Since, the case of unstable PDE is considered, the first eigenmode is used in the stabilizing condition given by Eq. 59. The constraints for the input and the state are $-3 \leq u(k) \leq 1$ and $-0.05 \leq z(0.5,k) \leq 0.3$.

It can be noticed that the model predictive control law for the infinite dimensional system achieves the input and state constraints satisfaction since the state evolution is exactly at the state constraint, see Figures 10–12. This confirms the previous findings in Refs. 21,22 in which the model predictive control was realized on the basis of an approximate model obtained by the Galerkin method with the PDE state constraints considered and realized as slack variables in the model predictive control law. Contrary to any previous published case where a linear PDE model is approximated with some type of the spatial discretization, the proposed model predictive control law for single scalar transport equation leads to an easy realizable constrained control algorithm formulation

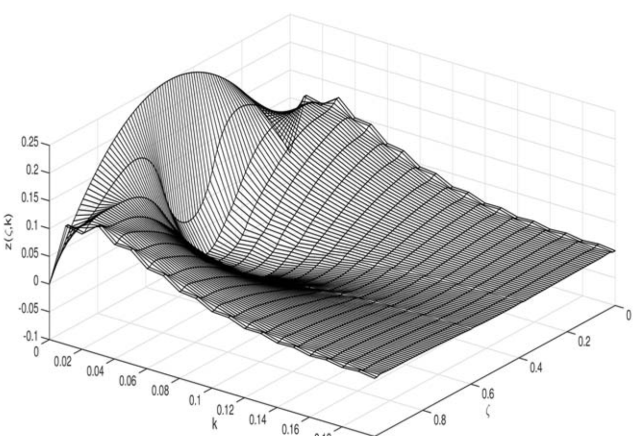

Figure 10. The evolution of the state profile under the model predictive control law Eq. 44 constructed using discrete time parabolic PDE system Eq. 4 with the Neumann boundary condition and input and state constraints.

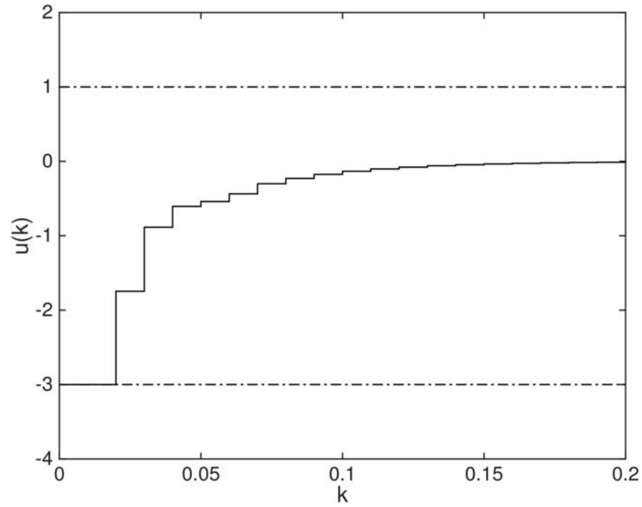

Figure 11. Input evolution profile under the model predictive control law Eq. 44 constructed using discrete time parabolic PDE system Eq. 4 with the Neumann boundary condition and input and state constraints (solid line); input constraints (dash-dot line).

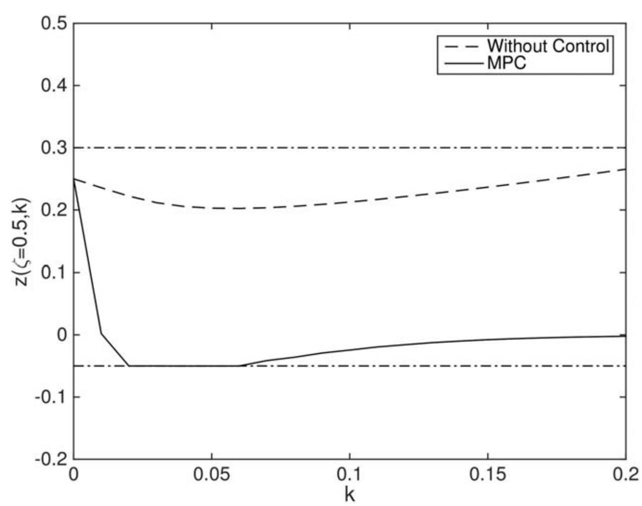

Figure 12. The comparison between profiles of closed-loop system under the implementation of the model predictive control law Eq. 44 constructed using discrete time parabolic PDE system Eq. 4 with the Neumann boundary condition and input and state constraints (solid line) and profile of open-loop system (dashed line); state constraints (dash-dot line).

which is not more complex than one when algorithms are dealing with the scalar finite dimensional models.

Summary

In summary, finite dimensional and computationally realizable model predictive control algorithms are developed in this work for a class of linear transport-reaction systems with consideration of input and state constraints arising in the context of a plug flow reactor and/or an axial dispersion reactor model. The dimensionless models described by hyperbolic PDE and/or parabolic PDE are explored and an exact time discretization algorithm is applied by introducing the Cayley-Tustin transform. The proposed discretization exactly maps from a continuous to a discrete infinite dimensional counterpart of the hyperbolic or parabolic PDE, and also preserves stability, controllability and observability properties of the system. The model predictive control formulation is developed in the inner product setting to account for the spatial nature of the problem, and various discrete models of hyperbolic PDE and/or parabolic PDE with different boundary conditions (Dirichlet, Neumann and Robin) are developed and used in the construction of the performance objective function, input and state constraints. Finally, the model predictive control laws are applied and if optimization is feasible, the controllers achieve the control objectives which are demonstrated via simulation studies. An important issue of stabilization in the case of linear unstable systems is addressed by the application of the terminal penalty condition. The following framework can be easily extended to the systems of linear parabolic and/or hyperbolic problems, and to the class of second order hyperbolic systems that model wave propagation phenomena, or more complex models of Kuramoto-Sivashinsky, Ginzburg Landau equations with boundary or/and in domain actuation or observation.

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Appendix A

One can easily demonstrate that the A_d operator takes the following form $Ad(\cdot)=[-I+2\delta[\delta-A]^{-1}](\cdot)$.

$$
\begin{aligned}
A_d z(\zeta,k-1) &= [\delta-A]^{-1}[\delta+A]z(\zeta,k-1)\\
&= [\delta-A]^{-1}\left[-v\frac{\partial z(\zeta,k-1)}{\partial\zeta}+(\psi+\delta)z(\zeta,k-1)\right]\\
&= \left[\int_0^\zeta \frac{1}{v}\left[-v\frac{\partial z(\eta,k-1)}{\partial\eta}+(\psi+\delta)z(\eta,k-1)\right]e^{-\frac{1}{v}\int_0^\eta(\psi-\delta)d\phi}d\eta\right]e^{\frac{1}{v}\int_0^\zeta(\psi-\delta)d\phi}\\
&= \left[\int_0^\zeta \frac{1}{v}\left[-v\frac{\partial z(\eta,k-1)}{\partial\eta}\right]e^{-\frac{1}{v}\int_0^\eta(\psi-\delta)d\phi}d\eta\right]e^{\frac{1}{v}\int_0^\zeta(\psi-\delta)d\phi}\\
&\quad+\left[\int_0^\zeta \frac{1}{v}[(\psi+\delta)z(\eta,k-1)]e^{-\frac{1}{v}\int_0^\eta(\psi-\delta)d\phi}d\eta\right]e^{\frac{1}{v}\int_0^\zeta(\psi-\delta)d\phi}\\
&= \left[\int_0^\zeta -e^{-\frac{1}{v}\int_0^\eta(\psi-\delta)d\phi}dz(\eta,k-1)\right]e^{\frac{1}{v}\int_0^\zeta(\psi-\delta)d\phi}\\
&\quad+\left[\int_0^\zeta \frac{1}{v}[(\psi+\delta)z(\eta,k-1)]e^{-\frac{1}{v}\int_0^\eta(\psi-\delta)d\phi}d\eta\right]e^{\frac{1}{v}\int_0^\zeta(\psi-\delta)d\phi}\\
&= \left[-e^{-\frac{1}{v}\int_0^\eta(\psi-\delta)d\phi}z(\eta,k-1)|_0^\zeta-\int_0^\zeta -z(\eta,k-1)d\left[e^{-\frac{1}{v}\int_0^\eta(\psi-\delta)d\phi}\right]\right]e^{\frac{1}{v}\int_0^\zeta(\psi-\delta)d\phi}\\
&\quad+\left[\int_0^\zeta \frac{1}{v}[(\psi+\delta)z(\eta,k-1)]e^{-\frac{1}{v}\int_0^\eta(\psi-\delta)d\phi}d\eta\right]e^{\frac{1}{v}\int_0^\zeta(\psi-\delta)d\phi}\\
&= \left[-e^{-\frac{1}{v}\int_0^\zeta(\psi-\delta)d\phi}z(\zeta,k-1)+z(0)-\int_0^\zeta \frac{1}{v}[(\psi-\delta)z(\eta,k-1)]e^{-\frac{1}{v}\int_0^\eta(\psi-\delta)d\phi}d\eta\right]e^{\frac{1}{v}\int_0^\zeta(\psi-\delta)d\phi}\\
&\quad+\left[\int_0^\zeta \frac{1}{v}[(\psi+\delta)z(\eta,k-1)]e^{-\frac{1}{v}\int_0^\eta(\psi-\delta)d\phi}d\eta\right]e^{\frac{1}{v}\int_0^\zeta(\psi-\delta)d\phi}\\
&= -z(\zeta,k-1)+2\delta\left[\left[\int_0^\zeta \frac{1}{v}z(\eta,k-1)e^{-\frac{1}{v}\int_0^\eta(\psi-\delta)d\phi}d\eta\right]e^{\frac{1}{v}\int_0^\zeta(\psi-\delta)d\phi}\right]\\
&= [-I+2\delta[\delta-A]^{-1}]z(\zeta,k-1)
\end{aligned}
$$

Appendix B

One can construct A_d^* of a hyperbolic PDE system as follows:

$$
\begin{aligned}
<A_d\Phi,\Psi^*> &= \int_0^L\left[-\Phi(\zeta)+2\delta\left[\int_0^\zeta \frac{1}{v}\Phi(\eta)e^{-\frac{1}{v}\int_0^\eta(\psi-\delta)d\phi}d\eta\right]e^{\frac{1}{v}\int_0^\zeta(\psi-\delta)d\phi}\right]\Psi^*(\zeta)d\zeta\\
&= \int_0^L -\Phi(\zeta)\Psi^*(\zeta)d\zeta+2\delta\int_0^L\left(\int_0^\zeta \frac{1}{v}\Phi(\eta)e^{-\frac{1}{v}\int_0^\eta(\psi-\delta)d\phi}d\eta\right)\Psi^*(\zeta)e^{\frac{1}{v}\int_0^\zeta(\psi-\delta)d\phi}d\zeta\\
&= \int_0^L -\Phi(\zeta)\Psi^*(\zeta)d\zeta+2\delta\int_0^L\int_0^\zeta \frac{1}{v}[\Phi(\eta)e^{-\frac{1}{v}\int_0^\eta(\psi-\delta)d\phi}][\Psi^*(\zeta)e^{\frac{1}{v}\int_0^\zeta(\psi-\delta)d\phi}]d\eta d\zeta\\
&= \int_0^L -\Phi(\zeta)\Psi^*(\zeta)d\zeta+2\delta\int_0^L\int_\eta^L \frac{1}{v}[\Phi(\eta)e^{-\frac{1}{v}\int_0^\eta(\psi-\delta)d\phi}][\Psi^*(\zeta)e^{\frac{1}{v}\int_0^\zeta(\psi-\delta)d\phi}]d\zeta d\eta\\
&= \int_0^L -\Phi(\zeta)\Psi^*(\zeta)d\zeta+2\delta\int_0^L\left(\int_\eta^L \frac{1}{v}\Psi^*(\zeta)e^{\frac{1}{v}\int_0^\zeta(\psi-\delta)d\phi}d\zeta\right)\Phi(\eta)e^{-\frac{1}{v}\int_0^\eta(\psi-\delta)d\phi}d\eta
\end{aligned}
$$

Interchanging the ζ and η, one obtains:

$$
\begin{aligned}
&<A_d\Phi,\Psi^*>\\
&= \int_0^L -\Phi(\zeta)\Psi^*(\zeta)d\zeta+2\delta\int_0^L\left(\int_\zeta^L \frac{1}{v}\Psi^*(\eta)e^{\frac{1}{v}\int_0^\eta(\psi-\delta)d\phi}d\eta\right)\Phi(\zeta)e^{-\frac{1}{v}\int_0^\zeta(\psi-\delta)d\phi}d\zeta\\
&= \int_0^L\left[-\Psi^*(\zeta)+2\delta\left[\int_\zeta^L \frac{1}{v}\Psi^*(\eta)e^{\frac{1}{v}\int_0^\eta(\psi-\delta)d\phi}d\eta\right]e^{-\frac{1}{v}\int_0^\zeta(\psi-\delta)d\phi}\right]\Phi(\zeta)d\zeta\\
&= <\Phi,A_d^*\Psi^*>
\end{aligned}
$$

Similarly, the construction of C_d^* for a hyperbolic PDE system is as follows:

$$<C_d\Phi,\Psi^*> = \int_0^L \left[\sqrt{2\delta}\left[\int_0^L \frac{1}{v}\Phi(\eta)e^{-\frac{1}{v}\int_0^\eta(\psi-\delta)d\phi}d\eta\right]e^{\frac{1}{v}\int_0^L(\psi-\delta)d\phi}\right]\Psi^*(\zeta)d\zeta$$

$$=\sqrt{2\delta}e^{\frac{1}{v}\int_0^L(\psi-\delta)d\phi}\int_0^L\int_0^L \frac{1}{v}\Phi(\eta)e^{-\frac{1}{v}\int_0^\eta(\psi-\delta)d\phi}\Psi^*(\zeta)d\eta d\zeta$$

$$=\sqrt{2\delta}e^{\frac{1}{v}\int_0^L(\psi-\delta)d\phi}\int_0^L\int_0^L \frac{1}{v}\Phi(\eta)e^{-\frac{1}{v}\int_0^\eta(\psi-\delta)d\phi}\Psi^*(\zeta)d\zeta d\eta$$

$$=\sqrt{2\delta}e^{\frac{1}{v}\int_0^L(\psi-\delta)d\phi}\int_0^L\left[\int_0^L \frac{1}{v}\Psi^*(\zeta)d\zeta\right]\Phi(\eta)e^{-\frac{1}{v}\int_0^\eta(\psi-\delta)d\phi}d\eta$$

$$=\sqrt{2\delta}e^{\frac{1}{v}\int_0^L(\psi-\delta)d\phi}\int_0^L\left[\int_0^L \frac{1}{v}\Psi^*(\eta)d\eta\right]\Phi(\zeta)e^{-\frac{1}{v}\int_0^\zeta(\psi-\delta)d\phi}d\zeta$$

$$=\int_0^L\left[\sqrt{2\delta}\left[\int_0^L \frac{1}{v}\Psi^*(\eta)d\eta\right]e^{-\frac{1}{v}\int_0^\zeta(\psi-\delta)d\phi}e^{\frac{1}{v}\int_0^L(\psi-\delta)d\phi}\right]\Phi(\zeta)d\zeta$$

$$=<\Phi, C_d^*\Psi^*>$$

Appendix C

One can obtain the construction of A_d^* for a parabolic PDE system with the Dirichlet boundary conditions as follows:

$$<A_d\Phi,\Psi^*> = \int_0^L\left[-\Phi(\zeta)+2\delta\left(\frac{1}{\sqrt{\delta-\psi}}\frac{\sinh(\sqrt{\delta-\psi}\zeta)}{\sinh(\sqrt{\delta-\psi}L)}\int_0^L\Phi(\eta)\sinh\left[\sqrt{\delta-\psi}(L-\eta)\right]d\eta\right.\right.$$

$$\left.\left.-\int_0^\zeta\frac{1}{\sqrt{\delta-\psi}}\Phi(\eta)\sinh\left[\sqrt{\delta-\psi}(\zeta-\eta)]d\eta\right)\right]\Psi^*(\zeta)d\zeta$$

$$=\int_0^L -\Phi(\zeta)\Psi^*(\zeta)d\zeta+2\delta\int_0^L\int_0^L\frac{1}{\sqrt{\delta-\psi}}\frac{\sinh(\sqrt{\delta-\psi}\zeta)}{\sinh(\sqrt{\delta-\psi}L)}\Phi(\eta)\Psi^*(\zeta)\sinh[\sqrt{\delta-\psi}(L-\eta)]d\eta d\zeta$$

$$-2\delta\int_0^L\int_0^\zeta\frac{1}{\sqrt{\delta-\psi}}\Phi(\eta)\Psi^*(\zeta)\sinh[\sqrt{\delta-\psi}(\zeta-\eta)]d\eta d\zeta$$

$$=\int_0^L -\Phi(\zeta)\Psi^*(\zeta)d\zeta+2\delta\int_0^L\int_0^L\frac{1}{\sqrt{\delta-\psi}}\frac{\sinh(\sqrt{\delta-\psi}\zeta)}{\sinh(\sqrt{\delta-\psi}L)}\Phi(\eta)\Psi^*(\zeta)\sinh[\sqrt{\delta-\psi}(L-\eta)]d\zeta d\eta$$

$$-2\delta\int_0^L\int_\eta^L\frac{1}{\sqrt{\delta-\psi}}\Phi(\eta)\Psi^*(\zeta)\sinh[\sqrt{\delta-\psi}(\zeta-\eta)]d\zeta d\eta$$

Interchanging the ζ and η leads to:

$$<A_d\Phi,\Psi^*>$$

$$=\int_0^L -\Phi(\zeta)\Psi^*(\zeta)d\zeta+2\delta\int_0^L\int_0^L\frac{1}{\sqrt{\delta-\psi}}\frac{\sinh(\sqrt{\delta-\psi}\eta)}{\sinh(\sqrt{\delta-\psi}L)}\Phi(\zeta)\Psi^*(\eta)\sinh[\sqrt{\delta-\psi}(L-\zeta)]d\eta d\zeta$$

$$-2\delta\int_0^L\int_\zeta^L\frac{1}{\sqrt{\delta-\psi}}\Phi(\zeta)\Psi^*(\eta)\sinh[\sqrt{\delta-\psi}(\eta-\zeta)]d\eta d\zeta$$

$$=\int_0^L\left[-\Psi^*(\zeta)+2\delta\left(\frac{1}{\sqrt{\delta-\psi}}\frac{\sinh[\sqrt{\delta-\psi}(L-\zeta)]}{\sinh(\sqrt{\delta-\psi}L)}\int_0^L\Psi^*(\eta)\sinh(\sqrt{\delta-\psi}\eta)d\eta\right.\right.$$

$$\left.\left.-\int_\zeta^L\frac{1}{\sqrt{\delta-\psi}}\Psi^*(\eta)\sinh[\sqrt{\delta-\psi}(\eta-\zeta)]d\eta\right)\right]\Phi(\zeta)d\zeta$$

$$=<\Phi, A_d^*\Psi^*>$$

Appendix D

When the boundary condition is a Neumann Boundary Condition, with the system resolvent operator described in Eq. 31, one can directly obtain the discrete time operators A_d, B_d, C_d and D_d of the parabolic system:

$$A_d(\cdot)=[-I+2\delta[\delta-A]^{-1}](\cdot)$$

$$=-(\cdot)+2\delta\left[\frac{1}{\sqrt{\delta-\psi}}\frac{\cosh(\sqrt{\delta-\psi}\zeta)}{\sinh(\sqrt{\delta-\psi})}\int_0^1(\cdot)\cosh[\sqrt{\delta-\psi}(1-\eta)\right]d\eta$$

$$-\int_0^{\zeta}\frac{1}{\sqrt{\delta-\psi}}(\cdot)\sinh[\sqrt{\delta-\psi}(\zeta-\eta)]d\eta] \tag{60}$$

$$B_d=\sqrt{2\delta}[\delta-A_{-1}]^{-1}B$$

$$=\sqrt{2\delta}\left[\frac{1}{\sqrt{\delta-\psi}}\frac{\cosh(\sqrt{\delta-\psi}\zeta)}{\sinh(\sqrt{\delta-\psi})}\int_0^1 B\cosh[\sqrt{\delta-\psi}(1-\eta)\right]d\eta$$

$$-\int_0^{\zeta}\frac{1}{\sqrt{\delta-\psi}}B\sinh[\sqrt{\delta-\psi}(\zeta-\eta)]d\eta] \tag{61}$$

$$C_d(\cdot)=\sqrt{2\delta}C[\delta-A]^{-1}(\cdot)$$

$$=\sqrt{2\delta}\left[\frac{1}{\sqrt{\delta-\psi}}\frac{\cosh(\sqrt{\delta-\psi}\zeta_0)}{\sinh(\sqrt{\delta-\psi})}\int_0^1(\cdot)\cosh[\sqrt{\delta-\psi}(1-\eta)\right]d\eta$$

$$-\int_0^{\zeta_0}\frac{1}{\sqrt{\delta-\psi}}(\cdot)\sinh[\sqrt{\delta-\psi}(\zeta_0-\eta)]d\eta] \tag{62}$$

$$D_d=C[\delta-A_{-1}]^{-1}B+D$$

$$=\frac{1}{\sqrt{\delta-\psi}}\frac{\cosh(\sqrt{\delta-\psi}\zeta_0)}{\sinh(\sqrt{\delta-\psi})}\int_0^1 B\cosh[\sqrt{\delta-\psi}(1-\eta)]d\eta \tag{63}$$

$$-\int_0^{\zeta_0}\frac{1}{\sqrt{\delta-\psi}}B\sinh[\sqrt{\delta-\psi}(\zeta_0-\eta)]d\eta$$

The expression of an adjoint operator A_d^* of a discrete operator A_d is in the following form:

$$A_d^*(\cdot)=-(\cdot)+2\delta\left[\frac{1}{\sqrt{\delta-\psi}}\frac{\cosh[\sqrt{\delta-\psi}(L-\zeta)]}{\sinh(\sqrt{\delta-\psi})}\right.$$

$$\int_0^1(\cdot)\cosh(\sqrt{\delta-\psi}\eta)d\eta \tag{64}$$

$$\left.-\int_{\zeta}^1\frac{1}{\sqrt{\delta-\psi}}(\cdot)\sinh[\sqrt{\delta-\psi}(\eta-\zeta)]d\eta\right]$$

The adjoint operator B_d^* is self-adjoint: $B_d^*=B_d$.

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