OPTIMAL TRANSITION CONTROL OF DIFFUSION-CONVECTION-REACTION PROCESSES

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Abstract: An approach for the optimal transition control of diffusion-convection-reaction processes based on finite-dimensional models is presented. The finite-dimensional state-space models are constructed directly from the process PDE through application of orthogonal collocation on finite elements in the spatial domain. The dimension of the derived state-space model can be further reduced using standard model reduction techniques. The optimal controller is designed based on the finite-dimensional state-space model using continuous-time linear quadratic regulator (LQR) techniques. *Copyright © 2007 IFAC*

Keywords: Diffusion-convection reaction process, model reduction, optimal transition control, orthogonal collocation

1. INTRODUCTION

Distributed chemical processes are naturally described by partial differential equations (PDEs) that are able to describe the spatiotemporal evolution of the process dynamics. Representative examples include chemical vapor deposition of semiconductor materials (Theodoropoulou *et al.*, 1998) and fluid flows (Graham *et al.*, 1999) etc. In order to develop accurate numerical solutions, the PDEs are usually converted to and solved as ordinary differential equations (ODEs) or algebraic equations using numerical methods like finite difference, finite element and finite volume (Liu and Jacobsen, 2004; Ammar *et al.*, 2006). Generally speaking, the resulting state-space model is of high dimension in order to precisely describe the spatial characteristics, especially when sharp gradients exist in the spatial domain. In order to develop dynamic optimization algorithms or feedback control systems suitable for real-time implementation, advanced model reduction techniques

such as Galerkin projection with empirical eigenfunctions, combination of Galerkin's method with approximate inertial manifolds, Krylov subspace and balanced truncation have been proposed to derive low-order ODEs with reasonable accuracy (Armaou and Christofides, 2002; Christofides, 2001). The controller is then designed based on the resulting reduced-order models, resulting in a significant reduction in computational effort.

In this work, we will present an optimal control approach for diffusion-convection-reaction processes using reduced-order models. In this case, a number of high-order Lagrange interpolation polynomials are applied on a finite number of collocation elements in the spatial domain to directly derive a low-dimensional differential-algebraic equation (DAE) model (Quarteroni and Valli, 1997). Such a DAE can be converted to a continuous-time state-space model by incorporating the boundary conditions into the ODEs in the spatial domain. If necessary, the dimension of the derived state-space model can be further reduced using model reduction techniques. In either case,

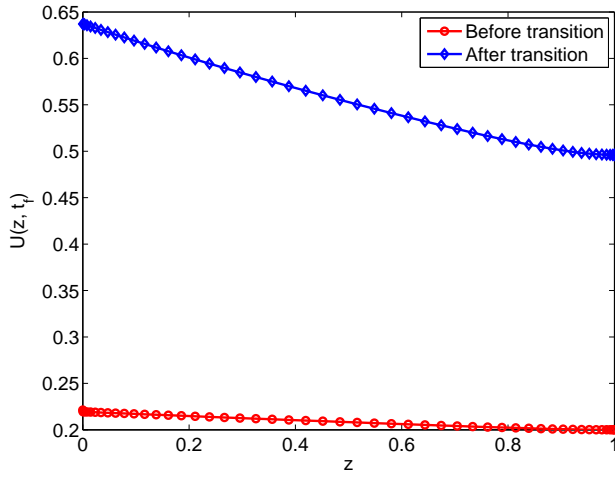[1] Corresponding author (e-mail: pdc@seas.ucla.edu)

Fig. 1. Steady-state spatial profiles of the concentration before transition and after transition.

the optimal control laws are designed based on the finite-dimensional models or their linearized forms using continuous-time linear quadratic regulator (LQR) control techniques.

The proposed method is applied to a concentration transition problem in an isothermal dispersed tubular reactor. The concentration transition problem is an important subject at the interface of reactor engineering and process control. This type of problem arises in modern chemical plants which generally make various products that differ in composition only in order to satisfy the needs of different customers. Representative industrial examples include grade transition in polyethylene plants (McAuley and Mac-Gregor, 1992; Cervantes *et al.*, 2002; Lo and Ray, 2006) and colored glass product transition in glass plants (Trier, 1987). In certain circumstances, a product transition may take days or weeks if the reactor is huge and the residence time of the reactor is large. A reduction of the transition time, which can be solved as an optimal control problem, can bring about significant economic benefits (Li and Christofides, 2007). In this work, we will focus on one type of concentration transition problem in which the grade of the final product is regulated through the concentration of a key component that is fed at the entrance of the reactor. If this key component to be controlled is not involved in any reactions, the transition process is described as a diffusion-convection process. If it does participate in any reaction, the process is a diffusion-convection-reaction process. In the remainder, we focus on the optimal transition control of a diffusion-convection-reaction process in which the key component is consumed following a second-order reaction.

2. MODEL CONSTRUCTION AND CONTROLLER DESIGN

2.1 Process model and spatial discretization

Consider an isothermal dispersed tubular chemical reactor with simultaneous convection, diffusion and a generic reaction. The evolution of concentration is described by the following PDE subject to the so-called Danckwerts boundary conditions (Danckwerts, 1953):

$$\frac{\partial U(z,t)}{\partial t} = -v\frac{\partial U(z,t)}{\partial z} + D\frac{\partial^2 U(z,t)}{\partial z^2} + R_a(U(z,t))$$

$$s.t. \quad vU(0^-,t) = vU(0^+,t) - D\frac{\partial U(z,t)}{\partial z}\mid_{z=0^+}$$

$$\frac{\partial U(z,t)}{\partial z}\mid_{z=L} = 0$$

$$(1)$$

where $U(0^-,t) = u(t)$ is the input variable, $U(L,t) = y(t)$ is the output variable and $R_a(z,t)$ is the reaction term ($R_a = -2KU^2$).

We solve the model of Eq.1 using orthogonal collocation. By applying the orthogonal collocation on N finite elements within the spatial domain, the primary variable $U(z,t)$ can be expressed as $U(z,t) = \sum_{i=1}^{N} l_i(z)U(z_i,t)$ at time t, where $l_i(z)$ is the Lagrange interpolation polynomial of $(N-1)$th order:

$$l_i(z) = \prod_{j=1,j\neq i}^{N} \frac{z-z_j}{z_i-z_j} \qquad (2)$$

which satisfies

$$l_i(z_j) = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases} \qquad (3)$$

Another important property of the Lagrange interpolation polynomials used in the orthogonal collocation approach is that they are orthogonal to each other, i.e.

$$\int_0^L l_i(z)l_j(z)dz = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases} \qquad (4)$$

Therefore, a small number of collocation points are required to obtain an accurate solution.

Based on the orthogonal collocation scheme, the collocation elements (z_i) and the Lagrange interpolation polynomial can be determined a priori without information from the structure of the PDE. Therefore, the partial derivatives of U with respect to the spatial coordinate can be expressed as follows:

$$\frac{\partial U(z,t)}{\partial z} = \sum_{i=1}^{N} U(z_i,t)\frac{dl_i(z)}{dz} \qquad (5)$$

$$\frac{\partial U^2(z,t)}{\partial z^2} = \sum_{i=1}^{N} U(z_i,t)\frac{d^2l_i(z)}{dz^2} \qquad (6)$$
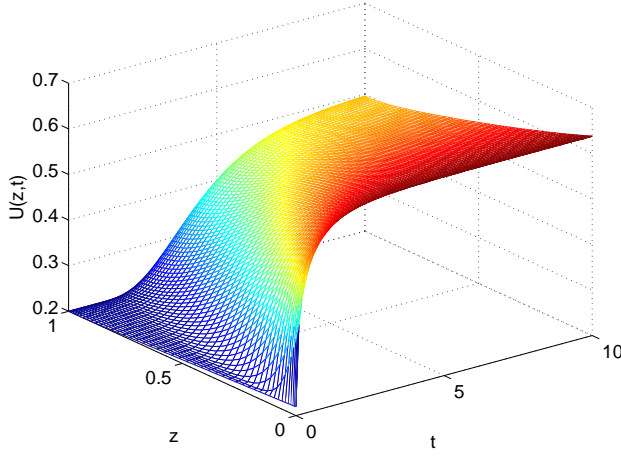
Fig. 2. Spatiotemporal distribution of the concentration during transition in the open-loop system.

Defining the two matrices:

$$\boldsymbol{A} = \left\{ A_{i,j} = \frac{dl_j(z_i)}{dz}; \ \ i,j = 1,2,...,N \right\} \quad (7)$$

and

$$\boldsymbol{B} = \left\{ B_{i,j} = \frac{dl_j^2(z_i)}{dz^2}; \ \ i,j = 1,2,...,N \right\} \quad (8)$$

the original PDE of Eq.1 can be converted to a set of ODEs:

$$\frac{dU(z_2,t)}{dt} = -v\sum_{j=1}^{N} A_{2,j}U(z_j,t) + D\sum_{j=1}^{N} B_{2,j}U(z_j,t)$$
$$+R_a(U(z_2,t))$$
$$\vdots$$
$$\frac{dU(z_{N-1},t)}{dt} = -v\sum_{j=1}^{N} A_{N-1,j}U(z_j,t)$$
$$+D\sum_{j=1}^{N} B_{N-1,j}U(z_j,t) + R_a(U(z_{N-1},t))$$

$$(9)$$

subject to the following boundary conditions:

$$vu(t) = vU(z_1,t) - D\sum_{j=1}^{N} A_{1,j}U(z_j,t)$$
$$\sum_{j=1}^{N} A_{N,j}U(z_j,t) = 0 \quad (10)$$

The system of Eqs.9-10 is a DAE of index one which can be further simplified by incorporating the boundary conditions into the ordinary differential equation. First, we rewrite the equations describing the boundary conditions in the following form:

$$(v - DA_{1,1})U(z_1,t) - DA_{1,N}U(z_N,t) =$$
$$D\sum_{j=2}^{N-2} A_{1,j}U(z_j,t) + vu(t)$$

$$A_{N,1}U(z_1,t) + A_{N,N}U(z_N,t) = -\sum_{j=2}^{N-2} A_{N,j}U(z_j,t)$$

$$(11)$$

and then define the following matrices and vectors:

$$\boldsymbol{A_d} = \left\{ A_{r_{i,j}} = A_{i+1,j+1}; \ \ i,j = 1,2,...,N-2 \right\}$$
$$\boldsymbol{B_d} = \left\{ B_{r_{i,j}} = B_{i+1,j+1}; \ \ i,j = 1,2,...,N-2 \right\}$$

$$\boldsymbol{A_b} = \begin{bmatrix} A_{2,1} & A_{2,N} \\ \vdots & \vdots \\ A_{N-1,1} & A_{N-1,N} \end{bmatrix}$$

$$\boldsymbol{B_b} = \begin{bmatrix} B_{2,1} & B_{2,N} \\ \vdots & \vdots \\ B_{N-1,1} & B_{N-1,N} \end{bmatrix}$$

$$\boldsymbol{M} = \begin{bmatrix} v - DA_{1,1} & -DA_{1,N} \\ A_{N,1} & A_{N,N} \end{bmatrix}$$

$$\boldsymbol{V} = \begin{bmatrix} v \\ 0 \end{bmatrix}$$

$$\boldsymbol{N} = \begin{bmatrix} DA_{1,2} & \cdots & DA_{1,N-1} \\ -A_{N,2} & \cdots & -A_{N,N-1} \end{bmatrix}$$

$$\boldsymbol{H} = \begin{bmatrix} 0 & 1 \end{bmatrix}$$

$$\boldsymbol{x} = [U(z_2,t) \ U(z_3,t) \ ... \ U(z_{N-1},t)]^T$$
$$\boldsymbol{d} = [U(z_1,t) \ U(z_N,t)]^T$$
$$\boldsymbol{f} = [R_a(U(z_2,t)) \ R_a(U(z_3,t)) \ ... \ R_a(U(z_{N-1},t))]^T$$

$$(12)$$

Using the above definitions, we have that:

$$\boldsymbol{d} = \boldsymbol{M}^{-1}\boldsymbol{N}\boldsymbol{x} + \boldsymbol{M}^{-1}\boldsymbol{V}u \quad (13)$$

provided that $\boldsymbol{M}$ is nonsingular. Using the above notation, Eqs.9-10 can be then written as

$$\dot{\boldsymbol{x}} = (-v\boldsymbol{A_d} + D\boldsymbol{B_d})\boldsymbol{x} + (-v\boldsymbol{A_b} + D\boldsymbol{B_b})\boldsymbol{d} + \boldsymbol{f}(\boldsymbol{x})$$
$$= [(-v\boldsymbol{A_d} + D\boldsymbol{B_d}) + (-v\boldsymbol{A_b} + D\boldsymbol{B_b})\boldsymbol{M}^{-1}\boldsymbol{N}]\boldsymbol{x}$$
$$+\boldsymbol{f}(\boldsymbol{x}) + (-v\boldsymbol{A_b} + D\boldsymbol{B_b})\boldsymbol{M}^{-1}\boldsymbol{V}u$$

$$(14)$$

and

$$y = \boldsymbol{H}\boldsymbol{M}^{-1}\boldsymbol{N}\boldsymbol{x} + \boldsymbol{H}\boldsymbol{M}^{-1}\boldsymbol{V}u \quad (15)$$

which is in the standard state-state form of a nonlinear dynamic process:

$$\dot{\boldsymbol{x}} = \boldsymbol{A_c}\boldsymbol{x} + \boldsymbol{B_c}u + \boldsymbol{f}(\boldsymbol{x})$$
$$y = \boldsymbol{C_c}\boldsymbol{x} + \boldsymbol{D_c}u$$

$$(16)$$

where $\boldsymbol{A_c} = [(-v\boldsymbol{A_d} + D\boldsymbol{B_d}) + (-v\boldsymbol{A_b} + D\boldsymbol{B_b})\boldsymbol{M}^{-1}\boldsymbol{N}]$, $\boldsymbol{B_c} = (-v\boldsymbol{A_b} + D\boldsymbol{B_b})\boldsymbol{M}^{-1}\boldsymbol{V}$, $\boldsymbol{C_c} = \boldsymbol{H}\boldsymbol{M}^{-1}\boldsymbol{N}$, $\boldsymbol{D_c} = \boldsymbol{H}\boldsymbol{M}^{-1}\boldsymbol{V}$.

2.2 Optimal control using LQR

The optimal control problem for the nonlinear ODE system of Eq.16 can be solved using control vector parametrization or nonlinear programming of the discretized system. To circumvent the computational complexity, we focus on the linearized system around the open-loop steady-state. The linearized system works as a state estimator based on which the control action is calculated. Because both the open-loop nonlinear system and the linearized system are stable, the observer gain is set to be zero for simplicity.

Let $\tilde{\boldsymbol{x}} = \boldsymbol{x} - \boldsymbol{x}_s$, $\tilde{u} = u - u_s$, and $\tilde{y} = y - y_s$, the nonlinear system can be written as follows:

$$\dot{\tilde{\boldsymbol{x}}} = \boldsymbol{A_c}\tilde{\boldsymbol{x}} + \boldsymbol{B_c}\tilde{u} + \boldsymbol{f}(\tilde{\boldsymbol{x}} + \tilde{\boldsymbol{x}}_s) - \boldsymbol{f}(\boldsymbol{x}_s)$$
$$\tilde{y} = \boldsymbol{C_c}\tilde{\boldsymbol{x}} + \boldsymbol{D_c}\tilde{u} \tag{17}$$

which can be linearized around the steady-state using the Jacobian matrix $\boldsymbol{A_l} = \dfrac{\partial \boldsymbol{f}(\boldsymbol{x})}{\partial \boldsymbol{x}}|_{\boldsymbol{x}=\boldsymbol{x}_s}$ to obtain:

$$\dot{\tilde{\boldsymbol{x}}} = (\boldsymbol{A_c} + \boldsymbol{A_l})\tilde{\boldsymbol{x}} + \boldsymbol{B_c}\tilde{u}$$
$$\tilde{y} = \boldsymbol{C_c}\tilde{\boldsymbol{x}} + \boldsymbol{D_c}\tilde{u} \tag{18}$$

The LQR problem is to minimize the following functional:

$$\min_{u(t)} J = \int_0^\infty (\tilde{y}^2 + \epsilon^2 \tilde{u}^2)dt \tag{19}$$

and the solution is given by the state feedback law: $\tilde{\boldsymbol{u}} = -\boldsymbol{K}\tilde{\boldsymbol{x}}$, where $\boldsymbol{K} = \boldsymbol{R}^{-1}(\boldsymbol{B}^T\boldsymbol{S} + \boldsymbol{G}^T)$, and $\boldsymbol{S}$ is determined by the Riccati equation (Arnold and Laub, 1984):

$$(\boldsymbol{A_c} + \boldsymbol{A_l})^T\boldsymbol{S} + \boldsymbol{S}(\boldsymbol{A_c} + \boldsymbol{A_l})$$
$$-(\boldsymbol{S}\boldsymbol{B_c} + \boldsymbol{G})\boldsymbol{R}^{-1}(\boldsymbol{B_c}^T\boldsymbol{S} + \boldsymbol{G}^T) + \boldsymbol{Q} = 0 \tag{20}$$

where $\boldsymbol{Q} = \boldsymbol{C_c}^T\boldsymbol{C_c}$, $\boldsymbol{G} = \boldsymbol{C_c}^T\boldsymbol{D_c}$, and $\boldsymbol{R} = \boldsymbol{D_c}^T\boldsymbol{D_c} + \epsilon^2$.

Typically, the dimension of an approximate state-space model formulated using orthogonal collocation is substantially smaller than the one obtained by finite difference and can be used for controller design. Moreover, in case a large number of collocation points are needed, model reduction techniques can be used to derive a reduced-order state-space model from the orthogonal collocation model based on which the controller can be synthesized. Let $\boldsymbol{\Phi}$ be a matrix consisting of the first r eignfunctions, Eq.18 can be converted to the following form:

$$\dot{\tilde{\boldsymbol{a}}} = \boldsymbol{A_r}\tilde{\boldsymbol{a}} + \boldsymbol{B_r}\tilde{u}$$
$$\tilde{y} = \boldsymbol{C_r}\tilde{\boldsymbol{a}} + \boldsymbol{D_r}\tilde{u} \tag{21}$$

Table 1. Parameters used in the simulation of the diffusion-convection-reaction process.

v	0.2
L	1
D	0.02
N	50
k	0.05

where $\boldsymbol{A_r} = \boldsymbol{\Phi}^T(\boldsymbol{A_c} + \boldsymbol{A_l})\boldsymbol{\Phi}$, $\boldsymbol{B_r} = \boldsymbol{\Phi}^T\boldsymbol{B_c}$, and $\boldsymbol{C_r} = \boldsymbol{C}\boldsymbol{\Phi}$, and $\boldsymbol{D_r} = \boldsymbol{D_c}$. Therefore, the $(N-2)$th state-space model is reduced to an rth one through the Galerkin projection, which can be then used for controller design. The solution of this LQR problem is given by the state feedback law $\tilde{\boldsymbol{u}} = -\boldsymbol{K_r}\tilde{\boldsymbol{a}}$ following a similar approach to the one presented on the basis of the high-order model.

2.3 Results and discussion

The control problem is to make an optimal transition of the concentration at the exit of the reactor from 0.2 to 0.5. The parameters used in the simulations are listed in Table 1. To determine the concentration profile within the reactor before and after transition, the steady state form of Eq. 16 is solved:

$$0 = \boldsymbol{A_c}\boldsymbol{x_s} + \boldsymbol{B_c}u_s + \boldsymbol{f}(\boldsymbol{x_s})$$
$$y_s = \boldsymbol{C_c}\boldsymbol{x_s} + \boldsymbol{D_c}u_s \tag{22}$$

and the results are shown in Figures 1 and 2. The collocation elements are not uniformly distributed along the spatial domain. Instead, they are highly clustered in the region close to the boundaries. The nonlinearity of the problem can be easily verified by checking the steady-state profiles of the concentration before and after transition, which are not proportional to each other. A calculation of the input variable also shows that u_s increases from 0.22 to 0.66 in order to make an increase of y_s from 0.2 to 0.5.

The closed-loop spatiotemporal profile of the concentration during the transition process solved using $\epsilon^2 = 0.01$ is shown in Figure 3. One apparent difference between the open-loop system (Figure 2) and the closed-loop system (Figure 3) is that the concentration at the inlet of the reactor is not increasing all the time under optimal control. Instead, it increases initially and then decreases after reaching a peak. Because the original steady-state of both the original system and the linearized system is stable, the difference between these two states approaches zero as the time exceeds a certain value, which is shown in Figure 4. The profiles of the manipulated input and of the controlled output under optimal control are shown in Figures 5 and 6. It is seen that the transition
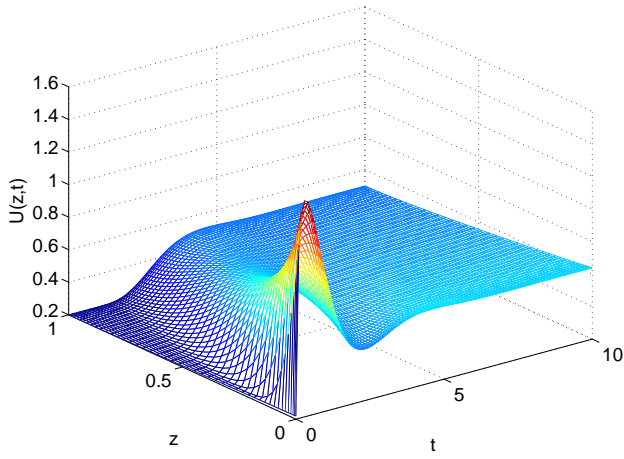
Fig. 3. Spatiotemporal distribution of the concentration during transition in the closed-loop system.
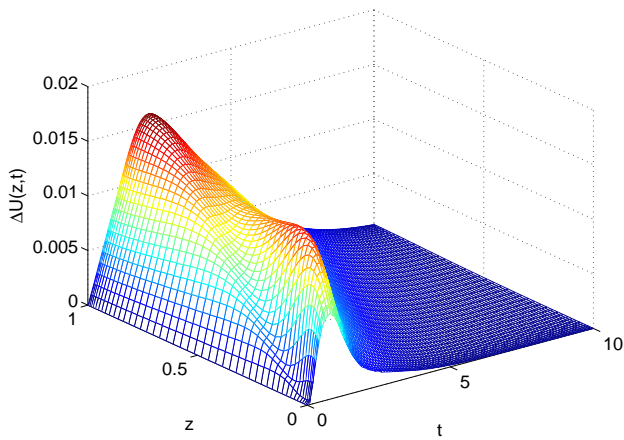

Fig. 4. Deviation of the closed-loop concentration profile calculated from the linearized model from the nonlinear system with the same control action.
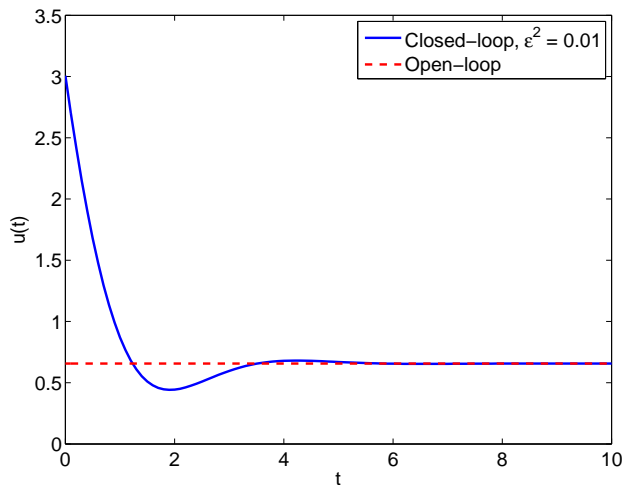

Fig. 5. Optimal trajectory of the manipulated input based on the high-dimensional state-space model derived from orthogonal collocation.
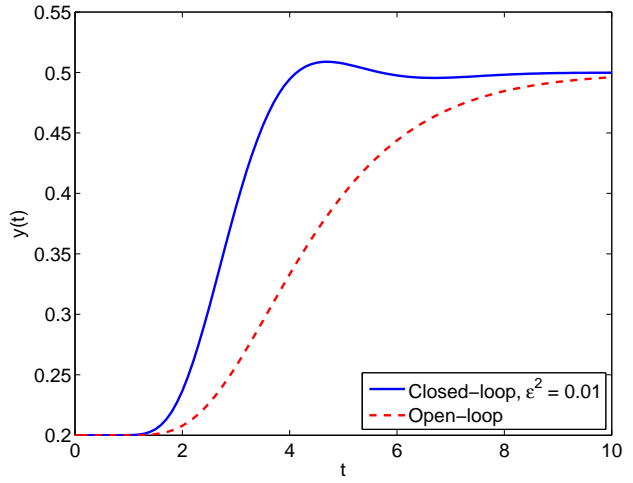

Fig. 6. Optimal trajectory of the controlled output using optimal control action calculated on the basis of the high-dimensional state-space model derived from orthogonal collocation.
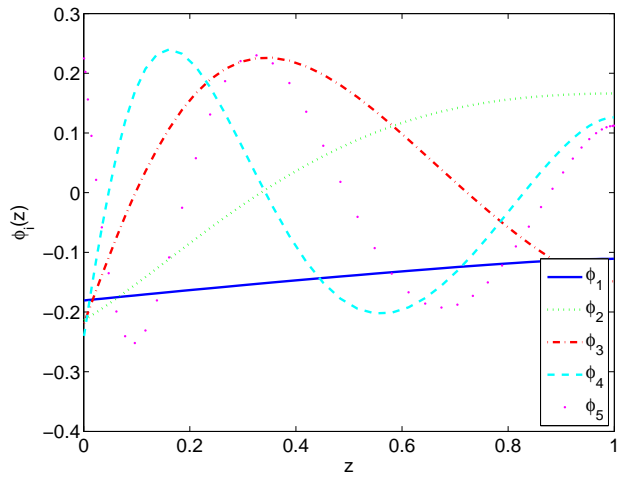

Fig. 7. First five empirical eigenfunctions for ensemble constructed from the high-dimensional model.
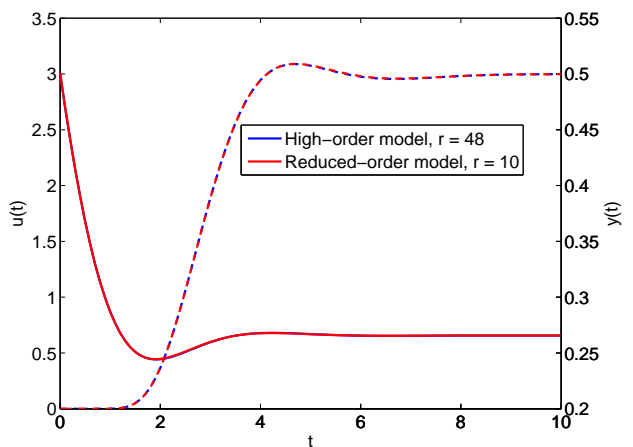

Fig. 8. Optimal trajectory of manipulated input and controlled output solved based on the reduced-order state-space model.
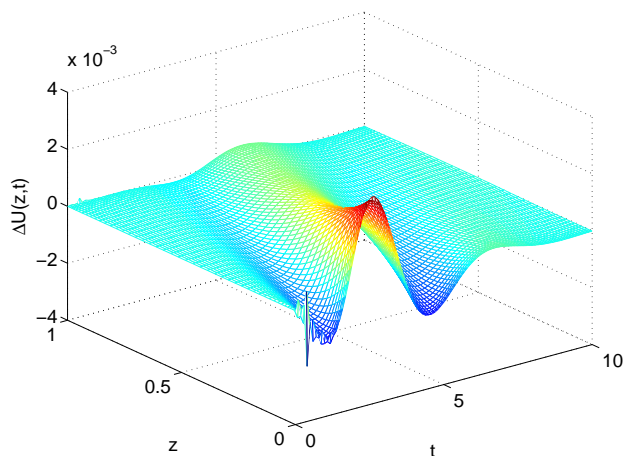
Fig. 9. Deviation of the closed-loop spatiotemporal concentration profile calculated using the reduced-order model ($r = 10$) from the high-dimensional model ($r = 48$) with the same control action.

time in the closed-loop system is significantly less than the one in the open-loop system.

In case the dimension of the finite-dimensional model formulated using the orthogonal collocation is high in order to accurately describe the process, a reduced-order model might be derived using proper orthogonal decomposition techniques for controller design. The SVD is first applied to an ensemble of the state variable $\boldsymbol{x}$ (a 48×101 matrix) to derive empirical eigenfunctions and it has been shown that the process can be described using about 10 empirical eigenfunctions with very reasonable accuracy. The first five eigenfunctions corresponding to the five largest eigenvalues λ_i is shown in Figure 7. The LQR problem is solved based on a 10th order model and the control action is fed to the high order nonlinear ODE model. The optimal trajectories of the manipulated input and controlled output are shown to be very close to those in which the control action is solved based on the high-order model (see Figure 8). A comparison of the spatiotemporal profile of the concentration based on the control action solved using the high-order model and the reduced-order model indicates that there is some small difference in the region close to the boundary in the beginning of the transition and in the whole region during the transition. However, even such a small difference becomes negligible when the process reaches steady state (see Figure 9).

3. ACKNOWLEDGEMENT

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