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ScienceDirect
Computers and Chemical Engineering 32 (2008) 2123–2135
Computers & Chemical Engineering
www.elsevier.com/locate/compchemeng

Optimal control of diffusion-convection-reaction processes using reduced-order models

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Received 24 July 2007; received in revised form 26 October 2007; accepted 26 October 2007
Available online 4 November 2007

Abstract

Two approaches for optimal control of diffusion-convection-reaction processes based on reduced-order models are presented. The approaches differ in the way spatial discretization is carried out to compute a reduced-order model suitable for controller design. In the first approach, the partial differential equation (PDE) that describes the process is first discretized in space and time using the finite difference method to derive a large number of recursive algebraic equations, which are written in the form of a discrete-time state-space model with sparse state, input and output matrices. Snapshots based on this high-dimensional state-space model are generated to calculate empirical eigenfunctions using proper orthogonal decomposition. The Galerkin projection with the computed empirical eigenfunctions as basis functions is then directly applied to the high-dimensional state-space model to derive a reduced-order model. In the second approach, a continuous-time finite-dimensional state-space model is constructed directly from the 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. In both cases, optimal controllers are designed based on the low-order state-space models using discrete-time and continuous-time linear quadratic regulator (LQR) techniques. The effectiveness of the proposed methods are illustrated through applications to a diffusion-convection process and a diffusion-convection-reaction process.

Keywords: Optimal control; Diffusion-convection-reaction processes; Model reduction; Empirical eigenfunctions; 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 (Armaou & Christofides, 1999; Li, Sopko, & McCamy, 2006; Lin & Adomaitis, 2001; Theodoropoulou, Adomaitis, & Zafiriou, 1998), thermal spray processing of coatings (Li & Christofides, 2005, 2006) and fluid flows (Baker, Armaou, & Christofides, 2000; Graham, Peraire, & Tang, 1999; Park & Jang, 2000; Rowley, Colonius, & Murray, 2004). 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 element and finite volume, etc. (e.g. Ammar, Ryckelynck, Chinesta, & Keunings, 2006; Broussely, Bertin, & Lagonotte, 2003; Kalkkuhl & Doring, 1993; Liu & Jacobsen, 2004). 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 & Christofides, 1999, 2000, 2002; Baker & Christofides, 2000; Baker et al., 2000; Bendersky & Christofides, 2000; Christofides, 2001; Christofides & Daoutidis, 1997; Park & Jang, 2000; Rowley et al., 2004; Shvartsman & Kevrekidis, 1998). The controller is

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doi:10.1016/j.compchemeng.2007.10.018

then designed based on the reduced-order models, resulting in a significant reduction in the time needed to compute the control action.

In this work, we will present two optimal control approaches for diffusion-convection-reaction processes using reduced-order models. In the first approach, the finite difference method is initially used and the PDE is converted to a large number of recursive algebraic equations. These algebraic equations are written in the form of discrete-time state-space models with sparse state, input and output matrices. Subsequently, snapshots based on the high-dimensional state-space model are generated to calculate empirical eigenfunctions using proper orthogonal decomposition. The Galerkin projection with the empirical eigenfunctions as basis functions is then directly applied to the high-dimensional state-space model to derive a low-order discrete-time state-space model. In the second approach, the finite-element based orthogonal collocation is used. 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 & 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 and the properties of the resulting ODE system allow, the dimension of the derived state-space model can be further reduced using model reduction techniques based on time-scale decomposition arguments. In either case, the optimal control laws are designed based on the low-dimensional state-space models or their linearized forms using discrete-time or continuous-time linear quadratic regulator (LQR) control techniques.

The proposed methods are applied to two concentration transition problems 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 a polyethylene plant (e.g. Cervantes, Tonelli, Brandolin, Bandoni, & Biegler, 2002; Lo & Ray, 2006; McAuley & MacGregor, 1992) and colored glass product transition in a glass plant (e.g. 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 & Christofides, 2007). In this work, we will focus on a 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, e.g. the transition of one colored glass product to another by regulating the colorant agent (key component) in the batch material which is then incorporated in the glass melt before exiting (Trier, 1987). If the 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 first focus on a diffusion-convection process and design an optimal controller on the basis of a reduced-order model constructed through Galerkin projection with empirical eigenfunctions as basis functions. Subsequently, we focus on a diffusion-convection-reaction process and design an optimal controller on the basis of a reduced-order model constructed through orthogonal collocation.

2. Optimal control of diffusion-convection processes

2.1. Control problem formulation

In this section, we focus on an isothermal dispersed tubular reactor in which the key component concentration is described by a parabolic PDE subject to the so-called Danckwerts boundary conditions (Danckwerts, 1953):

$$\frac{\partial U(z,t)}{\partial t} = -v\frac{\partial U(z,t)}{\partial z} + D\frac{\partial^2 U(z,t)}{\partial z^2}, \qquad \text{s.t.}$$
$$vU(0^-,t) = vU(0^+,t) - D\left.\frac{\partial U(z,t)}{\partial z}\right|_{z=0^+}, \quad \left.\frac{\partial U(z,t)}{\partial z}\right|_{z=L} = 0 \tag{1}$$

where $U(0^-,t) = u(t)$ is the inlet concentration (input variable), $U(L,t) = y(t)$ is the outlet concentration (output variable), t is the time, v is the fluid velocity in the reactor, L is the length of the reactor and D is the diffusion coefficient (or, more generally, dispersion coefficient). The control problem is to minimize the following functional:

$$\min_{u(t)} J = \int_0^\infty (y(t) - y_f)^2\,\mathrm{d}t + \epsilon^2 \int_0^\infty (u(t) - u_f)^2\,\mathrm{d}t \tag{2}$$

subject to the process dynamics described in Eq. (1), where u_f and y_f are the steady-state concentration of the key component at the inlet and outlet of the reactor after transition, and ϵ represents the weight on the control action during the transition process. Due to the linear nature of the process and the fact that all the molecules fed to the process will eventually flow out, the concentration transition problem can be converted to a dimensionless form in which the dimensionless concentration before and after transition is 0 and 1, respectively (Li & Christofides, 2007).

2.2. Spatial and temporal discretization of the PDE model

We first employ a standard finite difference discretization of the PDE of Eq. (1) in both time and space to obtain an accurate solution. Specifically, using the explicit finite difference approach with the forward time and center space (FTCS) scheme, the PDE of Eq. (1) can be written as the following set of algebraic equations:

$$\frac{U(z_i,t_{j+1}) - U(z_i,t_j)}{\Delta t} = -v\frac{U(z_{i+1},t_j) - U(z_{i-1},t_j)}{2\Delta z}$$