Chemical Engineering Science 138 (2015) 673–684

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

Dynamic shaping of transport–reaction processes with a combined sliding mode controller and Luenberger-type dynamic observer design

Davood Babaei Pourkargar, Antonios Armaou *

Department of Chemical Engineering, The Pennsylvania State University, University Park, PA 16802, United States

HIGHLIGHTS

- The dynamic shaping of transport–reaction processes is investigated.
- The spatiotemporal shaping is addressed via model order reduction.
- The desired spatiotemporal behavior is described by a target PDE.
- A sliding mode controller design is applied to track desired dynamics.
- A dynamic observer is employed to estimate the system dominant modes.

ARTICLE INFO

Article history:
Received 4 March 2015
Received in revised form
26 June 2015
Accepted 29 July 2015
Available online 15 August 2015

Keywords:
Dynamic shaping
Distributed parameter systems
Model order reduction
Sliding mode control
Dynamic observer
Process control

ABSTRACT

We focus on shaping the long-term spatiotemporal dynamics of transport–reaction processes which can be described by semi-linear partial differential equations (PDEs). The dynamic shaping problem is addressed via error dynamics regulation between the governing PDE and a target PDE which describes the desired spatiotemporal behavior. A model order reduction methodology is utilized to construct the required reduced order models (ROMs) for governing and target dynamics via Galerkin's method. We subtract the governing from the target ROMs to obtain reduced offset dynamics error. Then an output feedback sliding mode control structure is synthesized to stabilize the reduced error dynamics and correspondingly synchronize the system and the target spatiotemporal behaviors. A Luenberger-type dynamic observer is applied to estimate the states of the governing ROM required by the sliding mode controller. The proposed approach is applied to address the thermal spatiotemporal dynamic shaping problem in a tubular chemical reactor.

1. Introduction

Recently there has been an increasing focus on modeling and control of distributed parameter systems (DPSs) in chemical process and advanced material production industries. Such type of systems frequently arise in a wide range of chemical processes, e.g., fixed and fluidized bed reactors, polymerization and crystallization processes, chemical vapor deposition systems and semiconductor manufacturing processes, due to the existence of diffusion, dispersion and convection mechanisms (Adomaitis, 2003; Christofides, 2000; Lin and Adomaitis, 2001; Ray, 1981; Theodoropoulou et al., 1998). It is imperative to tightly control these processes so that there are zero product quality excursions, even when the process objectives dynamically change which is a usual occurrence in such industrial applications. While DPSs can be mathematically described by partial differential equations (PDEs) and the control problem is a difficult task due to the spatial distribution of the system states (Bohm et al., 1998; Christofides, 2000; Curtain and Zwart, 1995; Krstic and Smyshlyaev, 2008; Ng and Dubljevic, 2012; Smyshlyaev and Krstic, 2010), it becomes even more complicated in the case of chemical DPSs where chemical reactions take place leading to nonlinearities in the governing equation.

Focusing on transport–reaction processes with significant diffusive mechanisms and their mathematical description, we note that they can be described by semi-linear dissipative PDEs whose infinite-dimensional representation in an appropriate functional subspace can be partitioned into two subsystems: slow (and possibly unstable) and fast (and stable), with a time scale dynamic separation (Christofides, 2000). Considering such property, model order reduction (MOR) methodologies have been extensively used in modeling and control of chemical DPSs (Babaei Pourkargar and Armaou, 2014b, 2015b,c; Balas, 1991; Bentsman and Orlov, 2001; Christofides, 2000; Dubljevic et al., 2004; El-Farra et al., 2003; Hanczyc and Palazoglu, 1995). Galerkin's method is one of the typical approaches to implement MOR. The required basis functions

* Corresponding author. Tel.: +1 814 865 5316; fax: +1 814 865 7846.
E-mail address: armaou@engr.psu.edu (A. Armaou).

http://dx.doi.org/10.1016/j.ces.2015.07.054

in such approach can only be computed analytically if and only if the spatial differential operator is linear and the process operates over regular domains. Statistical approaches can be employed as an alternative solution to compute the empirical basis functions of a general class of DPSs from an ensemble of solution profiles. Proper orthogonal decomposition is one of the commonly used statistical techniques to find the optimal set of empirical basis functions for a representative set of solution data which has been widely applied in model reduction, optimization and control of DPSs (Armaou and Christofides, 2002; Babaei Pourkargar and Armaou, 2013b, 2014a; Izadi and Dubljevic, 2013; Sirovich, 1987) where geometric and Lyapunov based approaches have been used.

Sliding mode control is a variable structure nonlinear control method which changes the nonlinear system dynamics by applying a discontinuous control signal (Khalil, 2002; Slotine and Li, 1991). The sliding mode controller forces the system dynamics to slide along the boundaries of the system normal behavior called “sliding surface” (Edwards and Spurgen, 1998; Utkin, 1992). The discontinuous nature of the controller structure causes insensitivity to parameter variations and complete disturbance rejection (Bandyopadhyay and Janardhanan, 2006). Sliding mode optimization and controller designs have been applied in a wide range of chemical, mechanical and electrical systems (Bartolini et al., 1997; Bartoszewicz et al., 2008; Fridman, 2003; Hanczyc and Palazoglu, 1995; Misawa and Utkin, 2000).

To implement the model-reduced controller design for DPSs we need an accurate estimation of the states of the governing reduced order models (ROMs). Static observer designs, which were widely employed to estimate such desired states (Christofides, 2000; Dubljevic et al., 2004; Varshney et al., 2009), require the number of measurement sensors to be supernumerary to the number of ROM states. One of the solutions to circumvent such requirement is applying dynamic observers which theoretically need only one measurement sensor (Babaei Pourkargar and Armaou, 2013a,b; 2014c). While dynamic observer synthesis has reached an extensive maturity for lumped parameter systems described by ordinary differential equations (ODEs) (Gauthier et al., 1992; Karafyllis and Kravaris, 2005, 2012; Kazantzis and Kravaris, 1998; Keller, 1987; Michalska and Mayne, 1995; Soroush, 1997; Thau, 1995), the synthesis problem remains challenging for DPSs (Curtain et al., 2003; Fuji, 1980; Smyshlyaev and Krstic, 2005; Xu et al., 1995; Yang and Dubljevic, 2014).

In this paper we consider the spatiotemporal dynamic shaping of transport–reaction processes via MOR. The dynamic shaping problem is addressed by regulating the error dynamics between the governing PDE and a desired spatiotemporal dynamics which are described by a target PDE with the same spatial differential operator. The governing target PDEs are discretized by applying Galerkin's method to obtain ROMs in the form of low-dimensional modal ODEs when the required dominant basis functions are computed analytically by solving the eigenproblem of the linear part of the spatial differential operator. The error dynamics between the governing and target systems are derived by subtracting the ROMs in the form of low-dimensional ODEs which describe the spatiotemporal error dynamics. Then an output feedback control structure is synthesized to stabilize the error dynamics. The control structure is considered as a combination of a Lyapunov-based sliding mode controller (Khalil, 2002; Slotine and Li, 1991) and a Luenberger-type dynamic observer to estimate the system modes.

The remainder of the paper is organized as follows: a mathematical description of the studied class of semi-linear DPSs and their properties are presented in Section 2. Section 3 presents a short description of the used MOR method. The spatiotemporal dynamic shaping problem is addressed via an output feedback sliding mode control structure synthesis in Section 4. Finally, the proposed dynamic shaping method is successfully illustrated on thermal dynamic shaping inside a tubular chemical reactor described by a semi-linear PDE in Section 5.

2. Preliminaries

2.1. Problem formulation

To formulate the spatiotemporal dynamic shaping problem we consider a 1D transport–reaction process which can be described by a semi-linear PDE:

$$
\begin{aligned}
&\frac{\partial}{\partial t}X(z,t) = \mathcal{A}_n(z)X(z,t) + F(z,\ X(z,t)) + B(z)u(t),\\
&y(t) = \int_{\Omega} s(z)X(z,t)\,dz,\\
&q\left(X, \frac{\partial X}{\partial z}, \ldots, \frac{\partial^{n-1}X}{\partial z^{n-1}}\right) = 0 \quad \text{on } \partial\Omega,\\
&X(z,0) = X_0(z),
\end{aligned} \tag{1}
$$

where $X(z,t) \in \mathbb{R}$ is the spatiotemporal state of the system, $z \in \Omega$ the 1D spatial coordinate, t the time, Ω the process domain, $\partial\Omega$ the process boundaries, $\mathcal{A}_n(z)$ the linear spatial differential operator of order n, $F(z,\ X(z,t))$ the smooth Lipschitz nonlinear function, $u(t) \in \mathbb{R}^l$ the vector of manipulated inputs, $B(z)$ the spatial distribution of manipulated inputs, $y(t) \in \mathbb{R}^p$ the vector of contentious measurements, $s(z)$ the vector of measurements' spatial distribution, $q(X, \partial X/\partial z, \ldots, \partial^{n-1}X/\partial z^{n-1})$ the vector of linear homogeneous boundary conditions, and $X_0(z)$ the initial spatial profile of the system state. The dissipative PDE of (1) is linearly dominant, i.e., the spatial differential operator is purely linear and the nonlinearity only appears as a Lipschitz function in the system dynamics. Such equation arises in the majority of transport–reaction processes in the chemical process industries (Christofides, 2000; Ray, 1981), where the linear term of $\mathcal{A}_n(z)X(z,t)$ indicates the transport (diffusion, dispersion and convection) component and the nonlinear term of $F(z,\ X(z,t))$ expresses the reaction dynamics.

Remark 1. According to the Lipschitz property of the nonlinear function of $F(z,\ X(z,t))$ which makes it to be sufficiently smooth, the Picard–Lindelöf theorem can be applied to guarantee the existence and uniqueness of the solution (Teschl, 2012).

2.2. System representation

The studied DPS, which is described by the PDE of (1), can be represented in the abstract infinite-dimensional form of

$$
\begin{aligned}
&\dot{x}(t) = Ax(t) + f(x(t)) + bu(t), \qquad x(0) = x_0,\\
&y(t) = Sx(t),
\end{aligned} \tag{2}
$$

by defining the functional state of $x(t) \in \mathbb{W}$:

$$x(t) = X(\cdot, t),$$

the linear differential operator:

$$Ax(t) = \mathcal{A}(z)X(\cdot, t),$$

the nonlinear function:

$$f(x(t)) = F(z, X(\cdot, t)),$$

and the manipulated input operator:

$$bu(t) = B(z)u(t),$$

in an appropriate Sobolev subspace of $\mathbb{W}$:

$$\mathbb{W}(\Omega) = \left\{ \mathcal{H}, \frac{\partial \mathcal{H}}{\partial z}, \ldots, \frac{\partial^{n-1}\mathcal{H}}{\partial z^{n-1}} \in \mathcal{L}_2(\Omega) :\ q\left(\mathcal{H}, \frac{\partial \mathcal{H}}{\partial z}, \ldots, \frac{\partial^{n-1}\mathcal{H}}{\partial z^{n-1}}\right) = 0 \right\},$$