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Backstepping control of chemical tubular reactors

Dejan M. Bošković, Miroslav Krstić *

Department of Mechanical and Aerospace Engineering, University of California at San Diego, Mail code 0411, La Jolla, CA 92093-0411, USA

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Abstract

In this paper, a globally stabilizing boundary feedback control law for an arbitrarily fine discretization of a nonlinear PDE model of a chemical tubular reactor is presented. A model that assumes no radial velocity and concentration gradients in the reactor, the temperature gradient described by use of a proper value of the effective radial conductivity, a homogeneous reaction, the properties of the reaction mixture characterized by average values, the mechanism of axial mixing described by a single parameter model, and the kinetics of the first order is considered. Depending on the values of the nondimensional Peclet numbers, Damköhler number, the dimensionless adiabatic temperature rise, and the dimensionless activation energy, the coupled PDE equations for the temperature and concentration can have multiple equilibria that can be either stable or unstable. The objective is to stabilize an unstable steady state of the system using boundary control of temperature and concentration on the inlet side of the reactor. We discretize the original nonlinear PDE model in space using finite difference approximation and get a high order system of coupled nonlinear ODEs. Then, using backstepping design for parabolic PDEs we transform the original coupled system into two uncoupled target systems that are asymptotically stable in l^2-norm with appropriate homogeneous boundary conditions. In the real system, the designed control laws would be implemented through small variations of the prescribed inlet temperature and prescribed inlet concentration. The control design is accompanied by a simulation study that shows the feedback control law designed with sensing only on a very coarse grid (using just a few measurements of the temperature and concentration fields) can successfully stabilize the actual system for a variety of different simulation settings (on a fine grid).

Keywords: PDE model; Radial velocity; Nonlinear ODEs

1. Introduction

A feedback boundary control law that globally stabilizes an unstable steady state is designed for a chemical tubular reactor. The control is applied through variations of the inlet temperature and inlet concentration.

Due to the numerous industrial applications for chemical tubular reactors, the problem of monitoring and controlling them effectively is of great safety and economical importance. It has been shown numerically, analytically, and experimentally (see Hlaváek & Hofmann, 1970a and references therein) that in some cases the parabolic PDEs governing the temperature and concentration inside the tubular reactor can have more than one steady state solution. The multiple steady states can be either stable or unstable. The standard approach, once it was realized that there could be more than one steady state, was to find a priori estimates of the conditions under which there would be uniqueness or multiplicity. The obtained estimates would then be used to design the equipment such that undesired phenomena would be eliminated and the equipment operated rationally.

An alternative way to suppress the undesired behavior in chemical tubular reactors is through active control. Although the majority of the work on the control of chemical reactors was done for lumped parameter nonisothermal reactors (see Ray, 1981 and references therein), significant research efforts have focused on the analysis of the properties of PDE models for chemical tubular reactors (see Varma & Aris, 1977 for a survey), and more recently the analysis of existence and uniqueness of the state trajectories (Laabissi, Achhab, Winkin & Dochain, 2001). A large research activity has been

* Corresponding author. Tel.: +1-858-822-1374; fax: +1-858-822-3107; http://www.mae.ucsd.edu/research/krstic/

E-mail address: krstic@ucsd.edu (M. Krstić).

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also dedicated to the control designs based on PDE models of tubular reactors. One of the first results on the subject is due to Georgakis, Aris and Amundson (1977). More recently, using the fact that for parabolic PDE systems the eigenspectrum of the spatial differential operator can be partitioned into a finite-dimensional slow one and an infinite-dimensional stable fast one, Christofides (2001) used a combination of Galerkin's method with a procedure for the construction of approximate inertial manifolds for the derivation of ODE systems of dimension equal to the number of slow modes. The ODE systems obtained in this fashion yield solutions which are close, up to a desired accuracy, to the ones of the PDE system, for almost all times. These ODE systems were then used as the basis for the synthesis of output feedback controllers for nonisothermal tubular reactors that guarantee stability and enforce the output of the closed-loop system to follow, up to a desired accuracy, a prescribed response for almost all times. The distributed control was applied using the jacket temperature as the manipulated input. In a more recent paper by Orlov and Dochain (2001) a sliding mode control developed for minimum phase semilinear infinite-dimensional systems was applied to stabilization of chemical reactors (both plug flow and tubular). In that paper authors use distributed control to stabilize the system around prespecified temperature and concentration steady state profiles corresponding to a desired coolant temperature.

In this paper, we use the most general model of a chemical tubular reactor. The only assumptions made in the model are that the average velocity of reactant flow is constant, the dispersive fluxes of mass and heat follow a model with constant mass and energy dispersion coefficients, the heat transfered from any element of the jacket surrounding the reactor is proportional to the difference of the local temperature and the constant jacket temperature, and that the reaction rate at any point inside the domain is a nonlinear function of the temperature and concentration at that same point.

Our objective is to stabilize an unstable steady state using boundary control of temperature and concentration on the inlet side of the tubular reactor. To achieve that we first discretize the original PDE model in space using finite difference method which gives a high order system of coupled nonlinear ODEs for temperature and concentration. Then, using backstepping design (Krsti, Kanellakopoulos & Kokotovi, 1995), we obtain a discretized coordinate transformation that transforms the original coupled system into a target system consisting of two uncoupled systems that are asymptotically stable in l^2-norm with the same type of boundary conditions as the original system. The fact that the discretized coordinate transformation is invertible, for an arbitrary (finite) grid choice, implies *global asymptotic stability* of the discretized version of the original system. The coordinate transformation is then used to obtain nonlinear feedback boundary control laws for temperature and concentration in the original set of coordinates.

The paper is organized as follows. In Section 2 a PDE model for the chemical tubular reactor is derived and an overview of the stability properties for the case of multiple equilibrium profiles is presented. A nonlinear feedback control law that achieves global asymptotic stabilization of an unstable equilibrium profile is presented in Section 3, followed by the stability proof for the target system in Section 4. Finally, the feedback control law designed with sensing on a very coarse grid is shown to successfully stabilize the system for a variety of different simulation settings in a simulation study presented in Section 5.

2. Mathematical model

In this section, we derive a mathematical model for the chemical tubular reactor. A model that assumes no radial velocity and concentration gradients in the reactor, the temperature gradient described by use of a proper value of the effective radial conductivity, a homogeneous reaction, the properties of the reaction mixture characterized by average values, the mechanism of axial mixing described by a single parameter model, and the kinetics of the first order is considered. The mass and energy balance equations for the tubular chemical reactor are in that case given by Varma and Aris (1977).

$$T_t(z,t) = \frac{\lambda_{ea}}{\rho C_p} T_{zz}(z,t) - VT_z(z,t) - \frac{\Delta H}{\rho C_p} k_0 C(z,t) e^{-E/RT} - \frac{4h}{d\rho C_p}(T(z,t) - T_w) \tag{1}$$

$$C_t(z,t) = D_{ma} C_{zz}(z,t) - VC_z(z,t) - k_0 C(z,t) e^{-E/RT}, \tag{2}$$

with boundary conditions:

$$\frac{\lambda_{ea}}{\rho C_p} T_z(0,t) = V(T(0,t) - T_{in}), \tag{3}$$

$$D_{ma} C_z(0,t) = V(C(0,t) - C_{in}) \tag{4}$$

$$\frac{\lambda_{ea}}{\rho C_p} T_z(L,t) = 0, \tag{5}$$

$$D_{ma} C_z(L,t) = 0 \tag{6}$$

In the above system $T > 0$ denotes temperature; $C > 0$ stands for concentration; V, the linear velocity; λ_{ea}, the axial energy dispersion coefficient; D_{ma}, the axial mass dispersion coefficient; ΔH, the reaction heat; ρ, the fluid density; C_p, the specific heat; k_0, the kinetic constant; E, the activation energy; R, the gas constant;

h, the wall heat transfer coefficient; d, the reactor diameter; $T_w > 0$, the coolant temperature; $T_{in} > 0$, the inlet temperature; $C_{in} > 0$, the inlet reactant concentration and subscripts denote partial derivatives with respect to the corresponding variables.

Introducing nondimensional spatial variable, time, and nondimensional temperature, coolant temperature, and concentration, respectively, as:

$$z' = \frac{z}{L}, \tag{7}$$

$$t' = \frac{V}{L}t, \tag{8}$$

$$\theta(z', t') = \frac{E}{RT_{in}} \frac{T(z', t') - T_{in}}{T_{in}}, \tag{9}$$

$$\theta_c(z', t') = \frac{E}{RT_{in}} \frac{T_w(z', t') - T_{in}}{T_{in}}, \tag{10}$$

$$y(z', t') = \frac{C_{in} - C(z', t')}{C_{in}}, \tag{11}$$

and omitting superscripts' for convenience, we obtain a nondimensionalized system:

$$\theta_t(z, t) = \frac{1}{Pe_\theta}\theta_{zz}(z, t) - \theta_z(z, t) + BD_a(1 - y(z, t))e^{\theta/(1+\varepsilon\theta)} - \delta(\theta(z, t) - \theta_c) \tag{12}$$

$$y_t(z, t) = \frac{1}{Pe_y} y_{zz}(z, t) - y_z(z, t) + D_a(1 - y(z, t))e^{\theta/(1+\varepsilon\theta)} \tag{13}$$

with boundary conditions:

$$\theta_z(0, t) = Pe_\theta\theta(0, t), \tag{14}$$

$$y_z(0, t) = Pe_y y(0, t), \tag{15}$$

$$\theta_z(1, t) = 0, \tag{16}$$

$$y_z(1, t) = 0, \tag{17}$$

where $Pe_\theta = \rho C_p LV/\lambda_{ea}$, $Pe_y = LV/D_{ma}$, $\delta = (4h/d)(L/\rho C_p V)$, $D_a = (k_0 L/V)e^{-(E/RT_{in})}$, $B = \{(-\Delta H)C_{in}/\rho C_p T_{in}\}(E/RT_{in})$, and $\varepsilon = RT_{in}/E$, respectively, stand for the Peclet number for heat transfer, Peclet number for mass transfer, dimensionless heat transfer parameter, Damköhler number, dimensionless adiabatic temperature rise, and dimensionless activation energy. For θ_c we may assume, without loss of generality, $\theta_c = 0$ (Hlaváek & Hofmann, 1970a). Depending on the values of the nondimensional Peclet numbers, Damköhler number, the dimensionless adiabatic temperature rise, and the dimensionless activation energy, the system (Eqs. (12)–(17)) can have multiple equilibria that can be either stable or unstable. For a particular case with $Pe_\theta = Pe_y = 6$, $B = 10$, $\varepsilon = 0.05$, $D_a = 0.05$, and $\delta = 0$ (adiabatic case) the above system has three equilibrium profiles (Hlaváek & Hofmann, 1970b). The temperature steady state profiles $\bar{\theta}(z)$ for that case are shown in Fig. 1. It can be shown for the case of an adiabatic tubular reactor with equal Peclet numbers (Varma & Aris, 1977) that if the system parameters are such that multiple steady states exist, then they are alternatively asymptotically stable and unstable, in the pattern s–u–s···s–u–s (s = asymptotically stable, u = unstable). The middle of the three steady state profiles in Fig. 1 is,

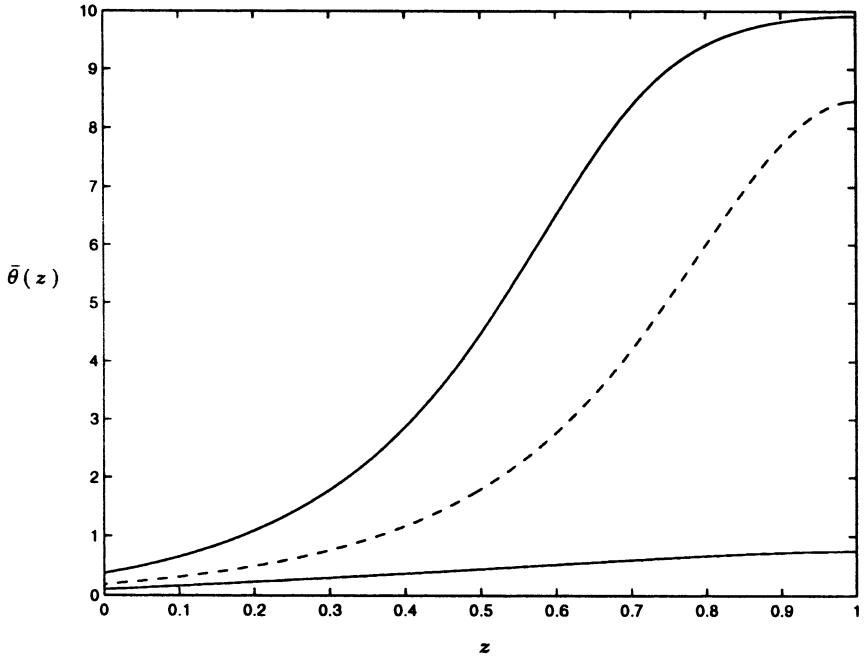

Fig. 1. Steady state temperature profiles for the adiabatic chemical tubular reactor with $Pe_\theta = Pe_y = 6$, $Da = 0.05$, $\varepsilon = 0.05$, and $B = 10$.

therefore, plotted with a dashed line to indicate that the steady state is unstable, while the outer two profiles plotted with solid lines are asymptotically stable.

Although not obvious from the Eqs. (12)–(17), it is physically justifiable to apply feedback boundary control at $z=0$ only. Since our backstepping control assumes that the control is applied at the one-end, we introduce new spatial, temperature and concentration variables, respectively, as $x=1-z$, $u(x,t)=\theta(1-z,t)-\bar{\theta}(1-z)$ and $v(x,t)=y(1-z,t)-\bar{y}(1-z)$, where $\bar{\theta}$ and $\bar{y}$ are the steady state solutions of the system (Eqs. (12)–(17)). We then have $\bar{u}(x)=\bar{\theta}(1-z)$ and $\bar{v}(x)=\bar{y}(1-z)$, and the system Eqs. (12)–(17) becomes:

$$u_t(x,t)=\frac{1}{Pe_\theta}u_{xx}(x,t)+u_x(x,t)+BD_{\mathrm{a}}g(u,v,\bar{u},\bar{v})-\delta u(x,t) \tag{18}$$

$$v_t(x,t)=\frac{1}{Pe_y}v_{xx}(x,t)+v_x(x,t)+D_{\mathrm{a}}g(u,v,\bar{u},\bar{v}), \tag{19}$$

where g is defined as:

$$g(u,v,\bar{u},\bar{v})=(1-v-\bar{v})\mathrm{e}^{(u+\bar{u}/1+\varepsilon(u+\bar{u}))}-(1-\bar{v})\mathrm{e}^{(\bar{u}/1+\varepsilon\bar{u})}, \tag{20}$$

with boundary conditions:

$$u_x(0,t)=0, \tag{21}$$

$$v_x(0,t)=0, \tag{22}$$

$$u_x(1,t)=-Pe_\theta u(1,t)+\Delta u_x(1,t), \tag{23}$$

$$v_x(1,t)=-Pe_y v(1,t)+\Delta v_x(1,t). \tag{24}$$

Note that the equilibrium of the system is now shifted to $(u,v)=(0,0)$. For the case when $\bar{\theta}$ and $\bar{y}$ (equivalently $\bar{u}$ and $\bar{v}$) are those corresponding to the unstable steady state, the equilibrium at the origin of the system (Eqs. (18)–(24)) is open loop ($\Delta u_x(1,t)=\Delta v_x(1,t)=0$) unstable. The objective is to stabilize $u(x,t)$ and $v(x,t)$ for that case by using $\Delta u_x(1,t)$ and $\Delta v_x(1,t)$ for control. In real application control would be implemented on the inlet side of the reactor through small variations of T_{in} and C_{in}. From a physical point of view this implies that the total temperature (concentration) control at the inlet side will consist of a prescribed component T_{in} (C_{in}) modulated by a control signal ΔT_{m} (ΔC_{m}).

3. Control law

To discretize the problem, let us start by denoting $h=1/N$, where N is an integer. Then, with u_i, v_i, $\bar{u}_i$, and $\bar{v}_i$, respectively, defined as $u_i(t)=u(ih,t)$, $v_i(t)=v(ih,t)$, $\bar{u}_i=\bar{u}(ih)$, and $\bar{v}_i=\bar{v}(ih)$, $i=0,\ldots,N$, we represent the nondimensional system Eqs. (18) and (19) as:

$$\dot{u}_i=\frac{1}{Pe_\theta}\frac{u_{i+1}-2u_i+u_{i-1}}{h^2}+\frac{u_{i+1}-u_i}{h}-\delta u_i+BD_{\mathrm{a}}g(u_i,v_i,\bar{u}_i,\bar{v}_i) \tag{25}$$

$$\dot{v}_i=\frac{1}{Pe_y}\frac{v_{i+1}-2v_i+v_{i-1}}{h^2}+\frac{v_{i+1}-v_i}{h}+D_{\mathrm{a}}g(u_i,v_i,\bar{u}_i,\bar{v}_i) \tag{26}$$

with boundary conditions at $x=0$ expressed as $(u_1-u_0)/h=0$ and $(v_1-v_0)/h=0$. We now suggest a backstepping controller which transforms the original system into the discretization of the system.

$$w_t(x,t)=\frac{1}{Pe_\theta}w_{xx}(x,t)+w_x(x,t)-C_1w(x,t) \tag{27}$$

$$s_t(x,t)=\frac{1}{Pe_y}s_{xx}(x,t)+s_x(x,t)-C_2s(x,t) \tag{28}$$

where $C_1>0$ and $C_2>0$, with homogeneous Neumann boundary conditions at $x=0$ given as $w_x(0,t)=s_x(0,t)=0$, and boundary conditions of a third kind at $x=1$ given as $w_x(1,t)=-Pe_\theta w(1,t)$ and $s_x(1,t)=-Pe_y s(1,t)$, which is asymptotically stable in l^2-norm. We should stress that the choice of the target system is one of the key issues. When transforming the original system we should try to keep its parabolic character, i.e. keep the second spatial derivative in the transformed coordinates. Even when applied for linear parabolic PDEs, the control laws obtained using standard backstepping would have gains that grow unbounded as $n\to\infty$. The problem with standard backstepping is that it would not only attempt to stabilize the equation, but also place all of its poles, and thus as $n\to\infty$, change its parabolic character. The coordinate transformation is sought in the form:

$$w_i=u_i-\alpha_{i-1}(u_1,\ldots,u_{i-1},v_1,\ldots,v_{i-1}) \tag{29}$$

$$s_i=v_i-\beta_{i-1}(u_1,\ldots,u_{i-1},v_1,\ldots,v_{i-1}) \tag{30}$$

where $w_i(t)=w(ih,t)$ and $s_i(t)=s(ih,t)$. The discretized form of Eqs. (27) and (28) is:

$$\dot{w}_i=\frac{1}{Pe_\theta}\frac{w_{i+1}-2w_i+w_{i-1}}{h^2}+\frac{w_{i+1}-w_i}{h}-C_1w_i \tag{31}$$

$$\dot{s}_i=\frac{1}{Pe_y}\frac{s_{i+1}-2s_i+s_{i-1}}{h^2}+\frac{s_{i+1}-s_i}{h}-C_2s_i \tag{32}$$

with $(w_1-w_0)/h=(s_1-s_0)/h=0$, $(w_N-w_{N-1})/h=-Pe_\theta w_N$, and $(s_N-S_{N-1})/h=-Pe_y s_N$.

By combining the above expressions, namely subtracting Eq. (31) from Eq. (25), expressing the obtained equation in terms of u_k-w_k, $k=i-1$, i, $i+1$, and applying Eq. (29) (analogously Eq. (32) from Eq. (26) for the concentration subsystem, and then using Eq. (30)) we obtain:

$$\alpha_i = \frac{1}{1+Pe_\theta h}\Bigg\{(2+Pe_\theta h + C_1 Pe_\theta h^2)\alpha_{i-1} - \alpha_{i-2} - (C_1-\delta)Pe_\theta h^2 u_i - Pe_\theta h^2 BD_a g(u_i, v_i, \bar{u}_i, \bar{v}_i) + Pe_\theta h^2 \frac{\partial \alpha_{i-1}}{\partial u_1}\Bigg[\frac{1}{Pe_\theta}\frac{u_2-u_1}{h^2} + \frac{u_2-u_1}{h} - \delta u_1 + BD_a g(u_1, v_1, \bar{u}_1, \bar{v}_1)\Bigg] + Pe_\theta h^2 \sum_{k=2}^{i-1}\frac{\partial \alpha_{i-1}}{\partial u_k}\Bigg[\frac{1}{Pe_\theta}\frac{u_{k+1}-2u_k+u_{k-1}}{h^2} + \frac{u_{k+1}-u_k}{h} - \delta u_k + BD_a g(u_k, v_k, \bar{u}_k, \bar{v}_k)\Bigg] + Pe_\theta h^2 \frac{\partial \alpha_{i-1}}{\partial v_1}\Bigg[\frac{1}{Pe_y}\frac{v_2-v_1}{h^2} + \frac{v_2-v_1}{h} + D_a g(u_1, v_1, \bar{u}_1, \bar{v}_1)\Bigg] + Pe_\theta h^2 \sum_{k=2}^{i-1}\frac{\partial \alpha_{i-1}}{\partial v_k}\Bigg[\frac{1}{Pe_y}\frac{v_{k+1}-2v_k+v_{k-1}}{h^2} + \frac{v_{k+1}-v_k}{h} + D_a g(u_k, v_k, \bar{u}_k, \bar{v}_k\Bigg]\Bigg\} \tag{33}$$

$$\beta_i = \frac{1}{1+Pe_y h}\Bigg\{(2+Pe_y h + C_2 Pe_y h^2)\beta_{i-1} - \beta_{i-2} - C_2 \mathrm{Pe}_y h^2 v_i - Pe_y h^2 D_a g(u_i, v_i, \bar{u}_i, \bar{v}_i) + Pe_y h^2 \frac{\partial \beta_{i-1}}{\partial u_1}\Bigg[\frac{1}{Pe_\theta}\frac{u_2-u_1}{h^2} + \frac{u_2-u_1}{h} - \delta u_1 + BD_a g(u_1, v_1, \bar{u}_1, \bar{v}_1)\Bigg] + Pe_y h^2 \sum_{k=2}^{i-1}\frac{\partial \beta_{i-1}}{\partial u_k}\Bigg[\frac{1}{Pe_\theta}\frac{u_{k+1}-2u_k+u_{k-1}}{h^2} + \frac{u_{k+1}-u_k}{h} - \delta u_k + BD_a g(u_k, v_k, \bar{u}_k, \bar{v}_k)\Bigg] + Pe_y h^2 \frac{\partial \beta_{i-1}}{\partial v_1}\Bigg[\frac{1}{Pe_y}\frac{v_2-v_1}{h^2} + \frac{v_2-v_1}{h} + D_a g(u_1, v_1, \bar{u}_1, \bar{v}_1)\Bigg] + Pe_y h^2 \sum_{k=2}^{i-1}\frac{\partial \beta_{i-1}}{\partial v_k}\Bigg[\frac{1}{Pe_y}\frac{v_{k+1}-2v_k+v_{k-1}}{h^2} + \frac{v_{k+1}-v_k}{h} + D_a g(u_k, v_k, \bar{u}_k, \bar{v}_k\Bigg]\Bigg\}, \tag{34}$$

starting with $\alpha_0 = \beta_0 = 0$. The controls are defined as:

$$\Delta u_x(1,t) = Pe_\theta \alpha_{N-1} + \frac{\alpha_{N-1}-\alpha_{N-2}}{h}, \tag{35}$$

$$\Delta v_x(1,t) = Pe_y \beta_{N-1} + \frac{\beta_{N-1}-\beta_{N-2}}{h}. \tag{36}$$

By inspection of the recursive control design algorithm one can verify that the coordinate transformation is invertible (which implies global asymptotic stability of the discretized system) and that the control law is smooth.

4. Asymptotic stability of the discretized system in modified coordinates

In this section we prove global asymptotic stability for Eqs. (27) and (28) with $w_x(0,t) = s_x(0,t) = 0$, $w_x(1,t) = -Pe_\theta w(1,t)$ and $s_x(1,t) = -Pe_y s(1,t)$ in L^2-norm. To prove the stability for the w-system we start with a Lyapunov function:

$$V_1 = \frac{1}{2}\int_0^1 w(x,t)^2 \mathrm{d}x \tag{37}$$

and find its derivative with respect to time, along the trajectories of the system Eq. (27), to be:

$$\begin{aligned}\dot{V}_1 &= \int_0^1 w w_t \mathrm{d}x = \int_0^1 \Bigg[\frac{1}{Pe_\theta} w_{xx} + w_x - C_1 w\Bigg] w \mathrm{d}x \\ &= \frac{1}{Pe_\theta}\Bigg[w w_x|_0^1 - \int_0^1 w_x^2 \mathrm{d}x\Bigg] + \frac{w^2}{2}\Bigg|_0^1 - C_1\int_0^1 w^2 \mathrm{d}x \\ &= -\frac{1}{2}(w^2(1)+w^2(0)) - \frac{1}{Pe_\theta}\int_0^1 w_x^2 \mathrm{d}x - C_1\int_0^1 w^2 \mathrm{d}x \\ &\le -2C_1 V_1,\end{aligned} \tag{38}$$

which implies that the system Eq. (27) with $w_x(0,t) = 0$ and $w_x(1,t) = -Pe_\theta w(1,t)$ is asymptotically stable in L^2-norm. The proof that Eq. (31) is asymptotically stable in l^2-norm with $(w_1 - w_0)/h = 0$ and $(w_N - w_{N-1})/h = -Pe_\theta w_N$ would be completely analogous. We would start with a Lyapunov function $V_{1d} = 1/2\ \Sigma_{t=0}^{N(t)} w_t^2$, follow the exactly same procedure, and obtain:

$$\dot{V}_{1d} \le -2C_1 V_{1d}. \tag{39}$$

The proof for the asymptotic stability of the s-system is completely analogous (the system equation and boundary conditions are of exactly the same form as for the w-system) and is, therefore, omitted.

5. Simulation study

In this section we present simulation results for a model of an adiabatic tubular reactor ($\delta = 0$) from Hlaváek and Hofmann (1970b) with $Pe_\theta = Pe_y = 6$, $D_a = 0.05$, $\varepsilon = 0.05$, and $B = 10$. For this particular choice of parameters the system has three equilibria. The equilibrium profiles for temperature are shown in Fig. 1. The equilibrium profiles for concentration have identical shape as the temperature ones, but with the amplitude scaled down with $1/B$ factor (see Hlaváek & Hofmann, 1970a for details), and are therefore, not shown separately. As shown in Hlaváek and Hofmann

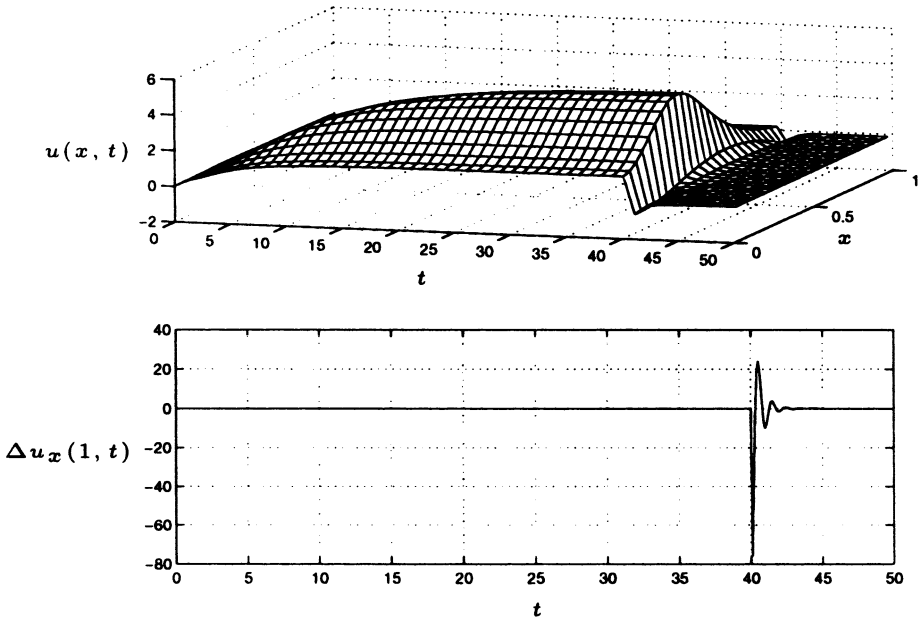

Fig. 2. Closed-loop temperature response with controller designed for $N_c = 2$, $C_1 = 3.5$, and $C_2 = 5$ (first row, $u(x, t)$; second row, the control effort $\Delta u_x(1, t)$).

(1970b), the middle profile is unstable while the outer two are stable. Our objective is to stabilize the unstable steady state using backstepping controller designed in Section 3.

As shown in Section 3, control laws for temperature Eq. (35) and concentration Eq. (36) are given in terms of α_{N-1}, α_{N-2}, and β_{N-1}, β_{N-2}, respectively, which can be easily obtained from the recursive expressions Eqs. (33) and (34) by using symbolic tools available. Once the final expressions for temperature and concentration control are obtained, for some particular choice of N, one would have to use full state feedback to stabilize the system, i.e. the complete knowledge of temperature and concentration fields is necessary. Instead, we show that controllers of relatively low order (designed with sensing on a much coarser grid) can successfully stabilize the system for a variety of different simulation settings.

The idea of using controllers designed using only a small number of steps of backstepping, or equivalently using only a small number of state measurements, to stabilize the system for a certain range of the open-loop instability is based on the fact that in most real life systems only a finite number of open-loop eigenvalues is unstable. Indeed, the simulation studies for the heat convection loop (Boskovic & Krstic, 2000) and solid rocket propellant burning instability suggest that low order backstepping controllers are capable of detecting the occurrence of instability from a limited number of measurements, and therefore, capable of successfully stabilizing the system for a variety of different simulation settings.

All simulations presented in this paper are run using BTCS finite difference method for $N = 200$ and the time step equal to 0.001 s. We start with a controller designed using only one step of backstepping, i.e. for $N_c = 2$, where the subscript 'c' stands for controller. From now on we will use N_c to refer to a coarse grid discretization used in controller design, i.e. N and h appearing in expressions Eqs. (33) and (34) will be replaced with N_c and $h_c = 1/N_c$, respectively, and N to refer to a fine grid used to simulate the behavior of the system described by equations Eqs. (25) and (26). The initial distribution used for this simulation is $u(x, 0) = 0.02(\bar{u}^{upp}(x) - \bar{u}^{mid}(x))$ and $v(x, 0) = 0.01(\bar{v}^{upp}(x) - \bar{v}^{mid}(x))$, where superscripts upp and mid refer to the upper (stable) and the middle (unstable) steady state, respectively. The motivation for using this type of initial profile, defined as a fraction of the difference between the two steady states, is motivated by a remark from Varma and Aris (1977). Applied to our system it says that for every perturbation that is in between the upper and the middle steady state profiles, the system goes to the upper one. Analogously, if we start between the middle and the lower one we will end up in the lower one. The system is initially perturbed for 2 and 1% of the difference between the upper and the middle temperature and concentration profiles, respectively. For the first 40 s we let the system evolve on its own and do not apply control. As it can be seen from Figs. 2 and 3, both temperature and concentration go to the upper stable equilibrium as the theory predicts. After 40 s the system has settled into the new steady state, and that is when we apply control. As it can be seen from

the same two figures, we successfully drive the system to the unstable steady state in a couple of nondimensional seconds. The controller used in this particular setting was designed with $C_1 = 3.5$ and $C_2 = 5$ and uses only one temperature and one concentration measurement at $x = 0.5$.

The situation is slightly different if we start in between the middle and the lower steady state. As it can be seen from Fig. 1, the distance between those two profiles is significantly bigger than the difference between the upper and the middle one, which will result in a more pronounced effect of the nonlinear terms. We can now stabilize the system only up to $u(x, 0) = 0.2(\bar{u}^{\text{low}}(x) - \bar{u}^{\text{mid}}(x))$ and $v(x, 0) = 0.2(\bar{v}^{\text{low}}(x) - \bar{v}^{\text{mid}}(x))$, where the superscript low refers to the lower (stable) steady state, using controller designed for $N_c = 2$. For example, it took controller 8 s to stabilize the system if both initial distributions were 15% of the difference between the two equilibrium profiles. A further increase in the size of the initial distributions resulted in much higher values for control gains C_1 and C_2 necessary to stabilize the system. The system also underwent a long period of an oscillatory behavior.

We now proceed to deriving control laws for $N_c = 3$ by introducing $h_c = 1/N_c$. Starting with $\alpha_0 = \beta_0 \equiv 0$ and using Eqs. (33) and (34) we find expressions for α_1, α_2, β_1 and β_2, and use those to find control laws Eqs. (35) and (36). The control signals depend on $u_i(t) = u(ih_c, t)$, and $v_i(t) = v(ih_c, t)$ for $i = 1, 2$ only, which means that we use only two temperature measurements u_1 at $x = 1/3$ and u_2 at $x = 2/3$, and corresponding two concentration measurements v_1 at $x = 1/3$ and v_2 at $x = 2/3$ to compute control laws.

As expected, by refining the grid in controller design from $N_c = 2$ to $N_c = 3$ we were able to extend the range of initial perturbations for which we can effectively stabilize the system. We are now able to stabilize the system when both initial distributions were 15% of the difference between the two equilibrium profiles in 2 s, as opposed to 8 *s* with the controller designed for $N_c = 2$. In fact, we can now stabilize the system even when the initial distribution is closer to the lower profile than it is to the middle one. The closed loop response of the system with initial perturbations in temperature and concentration $u(x, 0) = 0.5(\bar{u}^{\text{low}}(x) - \bar{u}^{\text{mid}}(x))$ and $v(x, 0) = 0.55(\bar{v}^{\text{low}}(x) - \bar{v}^{\text{mid}}(x))$, and control gains equal to $C_1 = 5$ and $C_2 = 2.5$ is shown in Figs. 4 and 5. As it can be seen, the controller successfully brings the system to the unstable equilibrium after a short period of oscillatory behavior. The controller designed for $N_c = 3$ was capable of stabilizing the system with even higher values of the initial perturbations, but it required much higher gains and system underwent a longer period of oscillatory behavior. We were not able though to recover the system from the lower steady state as we were able to in the case of the upper steady state.

In general, to accommodate the higher levels of initial disturbance one would have to increase the order of controller by applying recursive expressions Eqs. (33) and (34) for higher N_c. Designing controllers for higher N_c would help the controller extract more information about the disturbance and stabilize the system more effectively using smaller control gains. A similar type of pattern was also encountered in the case of the thermal

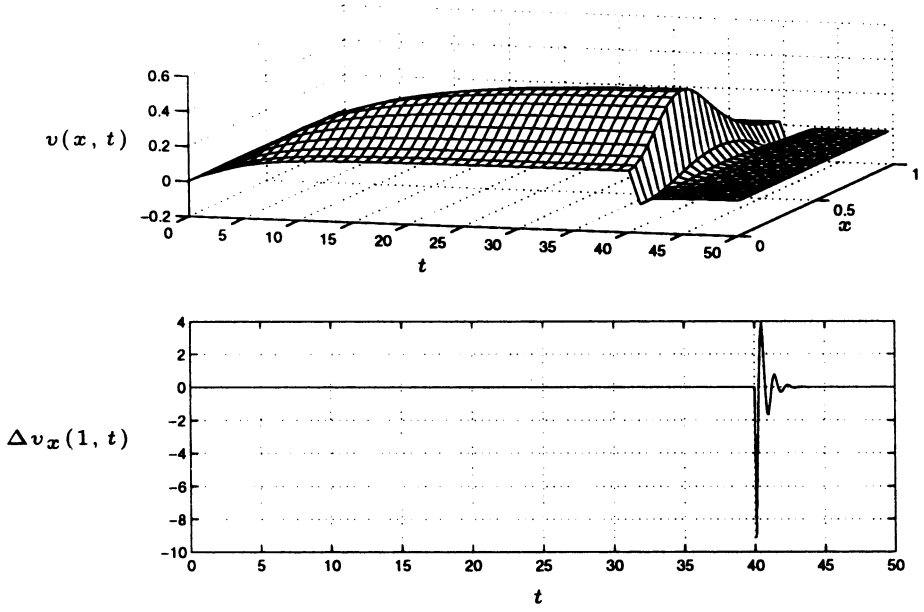

Fig. 3. Closed-loop concentration response with controller designed for $N_c = 2$, $C_1 = 3.5$, and $C_2 = 5$ (first row, $v(x, t)$; second row, the control effort $\Delta v_x(1, t)$).

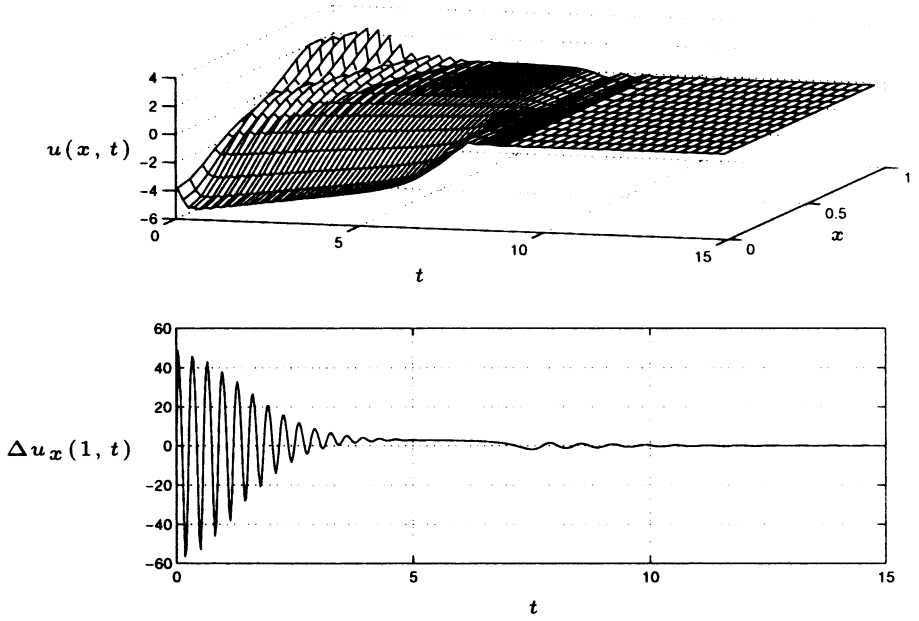

Fig. 4. Closed-loop temperature response with controller designed for $N_c = 3$, $C_1 = 5$, and $C_2 = 2.5$ (first row, $u(x, t)$; second row, the control effort $\Delta u_x(1, t)$).

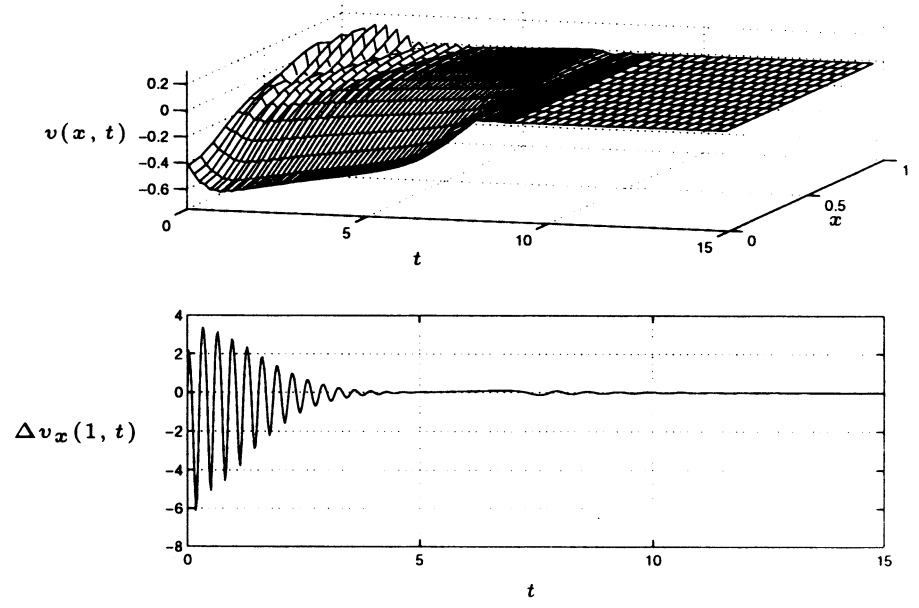

Fig. 5. Closed-loop concentration response with controller designed for $N_c = 3$, $C_1 = 5$ and $C_2 = 2.5$ (first row, $v(x, t)$; second row, the control effort $\Delta v_x(1, t)$).

convection loop (Boskovic & Krstic, 2000). The simulation results in Boskovic and Krstic (2000) suggested that to accommodate the flows with higher Rayleigh number one had to increase the order of controller.

6. Conclusions

A nonlinear feedback controller based on Lyapunov backstepping design that achieves global asymptotic stabilization of an unstable steady state for chemical tubular reactors has been derived. The result holds for any finite discretization in space of the original PDE model.

The simulation study indicates that a feedback control law designed using only couple of steps of backstepping can be successfully used to stabilize the system for a variety of different simulation settings. In particular, the controller designed using only one step of backstepping was capable of transferring the system

from one of the two stable steady states to the unstable one.

One key question presents a challenge for future research. It would be of interest to extend this result from the case of an arbitrary finite discretization of the model in space to the continuous model itself. This would, among other things, involve the proof that the proposed coordinate transformation remains bounded in the limit when the spatial grid becomes infinitely fine, i.e. when N tends to infinity. We intend to use the proof of boundedness for the linearized version of the tubular reactor model from Boskovic, Balogh and Krstic (2001) and try to extend the result to the original nonlinear model.

Another important question is whether a controller based on a sufficiently fine gridding would work on any grid finer than that for which it was designed. A partial answer to this question is in Boskovic et al. (2001) where weak continuity of backstepping feedback laws is shown for linearized PDE models. This result ensures that if the grid for control design is sufficiently fine, the control law does not change significantly during further grid refinements. However, the question of closed-loop stability with a controller designed on one grid and simulated on another grid is a challenging topic for future research.

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References

Boskovic, D., & Krstic, M. (2000). Nonlinear stabilization of a thermal convection loop by state feedback. *Automatica*, in press.

Boskovic, D., Balogh, A., & Krstic, M. (2001). Backstepping in infinite dimension for a class of parabolic distributed parameter systems. Submitted for publication.

Christofides, P. (2001). *Nonlinear and robust control of partial differential equation systems*: *methods and applications to transport–reaction processes* (p. 2001). Boston: Birkhäuser.

Georgakis, C., Aris, R., & Amundson, N. R. (1977). Studies in the control of tubular reactors. Parts I–III. *Chemical Engineering Science*, *32*, 1359–1387.

Hlaváek, V., & Hofmann, H. (1970a). Modeling of chemical reactors-XVI: steady state axial heat and mass transfer in tubular reactors—an analysis of the uniqueness of solutions. *Chemical Engineering Science*, *25*, 173–185.

Hlaváek, V., & Hofmann, H. (1970b). Modeling of chemical reactors-XVII: steady state axial heat and mass transfer in tubular reactors—numerical investigation of multiplicity. *Chemical Engineering Science*, *25*, 187–199.

Krsti, M., Kanellakopoulos, I., & Kokotovi, P. V. (1995). *Nonlinear and adaptive control design* (p. 1995). New York: Wiley.

Laabissi, M., Achhab, M. E., Winkin, J. J., & Dochain, D. (2001). Trajectory analysis of nonisothermal tubular reactor nonlinear models. *Systems and Control Letters*, *42*, 169–184.

Orlov, Y., & Dochain, D. (2001). Discontinuous feedback stabilization of minimum phase semilinear infinite–dimensional systems with applications to chemical tubular reactor. *IEEE Transactions on Automatic Control*, submitted for publication.

Ray, W. H. (1981). *Advanced process control*. New York: McGraw-Hill.

Varma, A., & Aris, R. (1977). Stirred pots and empty tubes. In L. Lapidus, & N. R. Amundson, *Chemical reactor theory* (pp. 79–154). Prentice-Hall.