BIFURCATION ANALYSIS OF INDEX INFINITY PARABOLIC MODELS DESCRIBING REACTORS AND REACTING FLOWS

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Abstract

We show that most steady-state models of chemical reactors and reacting flows in which convection effects are dominant and axial diffusion/conduction is neglected are not of parabolic type but are index infinity differential-algebraic equations that could have an infinite number of solutions. Standard numerical methods find only one of these solutions (corresponding to latest possible ignition). We present a complete bifurcation analysis of these models, a method for finding all solutions, determine the stability and, for some simpler cases, the domain of initial conditions attracted to these states.

Keywords

Parabolic models, differential-algebraic equations, multiple solutions, bifurcation and stability

Introduction

Mathematical models that describe the steady-state behavior of chemical reactors and reacting flows in which volumetric and/or wall reactions occur can be generally classified as elliptic or parabolic. The behavior of elliptic models is well studied in the literature and they are known to display a variety of solutions and bifurcations (e.g. multiple homogeneous solutions and various types of patterned/asymmetric solutions). In the literature, the so called "boundary layer models (in which axial diffusion/conduction is neglected) used to describe these systems are treated as parabolic equations and having a unique solution. Such a solution is usually obtained by discretization of the transverse coordinate and integration in the axial direction.

However, it was shown in our earlier work that boundary layer models of parabolic type are index infinity differential-algebraic equation (DAE) systems, and could have an infinite number of solutions. Further, the integration of such models along the flow direction (forward) and against the flow direction (backward) could lead to different solutions. In this work, we present further observations and analytical as well as numerical methods for determining the various solutions of such index infinity DAE systems. We consider three specific systems to illustrate the main ideas and techniques: (i) a DAE system consisting of one differential equation (in axial coordinate) and one algebraic equation, having infinite number of solutions (such a system is obtained by transverse averaging of the partial differential equation models) (ii) a parabolic equation in two variables (axial and transverse) that has nonlinearity in the boundary conditions (iii) a parabolic equation in two variables with linear boundary conditions but a nonlinear source term. For these cases, we present bifurcation analysis as well as numerical methods for determining all the solutions with particular emphasis on how to determine the physically relevant discontinuous solutions along with their stability.

Steady-state Reactor Models of Parabolic Type

As an example [of type (iii)], we consider the steady-state model describing the homogeneous tubular reactor (with negligible longitudinal diffusion/conduction). For the case of a single first-order reaction, this model can be expressed in dimensionless form as follows:

$$u(r)\frac{\partial c}{\partial \eta} = \nabla_{\perp}^{2} c - \phi^{2} c \ \exp\left[\frac{\theta}{1+\theta/\gamma}\right], \ 0 < r < 1, \eta > 0 \qquad (1a)$$

$$u(r)\frac{\partial \theta}{\partial \eta} = Le_{f}\nabla_{\perp}^{2}\theta + B\phi^{2} c \ \exp\left[\frac{\theta}{1+\theta/\gamma}\right], 0 < r < 1, \eta > 0 \qquad (1b)$$

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$$c\big|_{\eta=0}=1;\quad \theta\big|_{\eta=0}=0;\quad \frac{\partial c}{\partial r}\bigg|_{r=0,1}=0=\frac{\partial \theta}{\partial r}\bigg|_{r=0,1} \tag{1c}$$

where r and η are transverse and axial coordinates; $u(r)$ is the velocity profile; c and θ are concentration and temperature; $\nabla_{\perp}^{2}$ is transverse Laplacian operator; ϕ^2, Le_f, B and γ are Thiele modulus, Lewis number, adiabatic temperature rise and activation energy, respectively in dimensionless form. (Here, the axial coordinate $\eta=z/P=xD_m/a^2<u>$, where z is the dimensionless length along the tube and P is the transverse Peclet number).

A similar model may be written for describing the steady-state behavior of a catalytic tubular reactor. The main difference is that the non-linearity is present in the boundary conditions [type (ii)]. In the literature, these models are treated as parabolic models and are solved by discretizing the model in transverse coordinate and integrating in the axial direction. Such standard methods lead to a unique solution. However, these methods fail to capture other solutions that arise due to non-linear behavior. For example, discretizing the above model (Eq. 1), leads to at least one algebraic equation (coupled to differential equations in η) due to velocity vanishing at the wall. Therefore, these systems are differential-algebraic in nature and we show that they can have infinite number of solutions depending on the reaction parameters.

We use the Liapunov-Schmidt technique for transverse averaging of these models and reduce them to the following simpler form [type (i)]:

$$\frac{\partial \theta_m}{\partial \eta}=B\phi^2 R(\theta_s,c_s)=-B\frac{\partial c_s}{\partial \eta}=NuLe_f(\theta_s-\theta_m),\quad \eta>0 \tag{2a}$$

$$R(\theta_s,c_s)=\frac{\exp\left[\dfrac{\theta_s}{1+\theta_s/\gamma}\right]}{1+\dfrac{\phi^2}{Sh}\exp\left[\dfrac{\theta_s}{1+\theta_s/\gamma}\right]}c_s,\quad \eta>0 \tag{2b}$$

$$c_s\big|_{\eta=0}=1;\quad \theta_m\big|_{\eta=0}=0 \tag{2c}$$

where subscripts 's' and 'm' denote the cross-sectional (volumetric reaction) or peripheral averaged (wall reaction) and velocity-weighted transverse averaged quantities. Here, Nu and Sh are the Nusselt and Sherwood numbers, respectively.

Results and Discussion

Bifurcation analysis shows that the reduced order model (Eq. 2) may have index zero (initial value problem), one or infinity depending on the reaction parameters. Figure 1 shows a phase diagram with index and the type of solution(s) that could exist for one typical set of parameters: $\left(Le_f=1=Sh=Nu \text{ and } \gamma\to\infty\right)$. We note that in regions II and III, the index is infinity and the system has infinite number of discontinuous solutions.

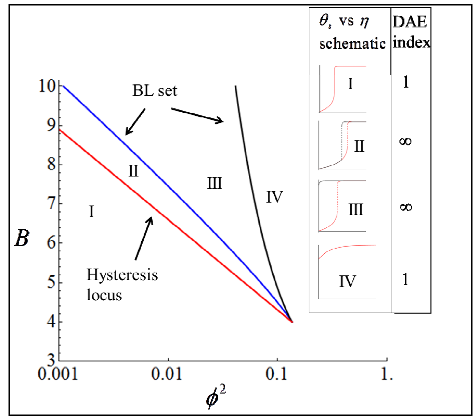

Figure 1. Phase diagram showing the index of DAE-system and the type of solutions

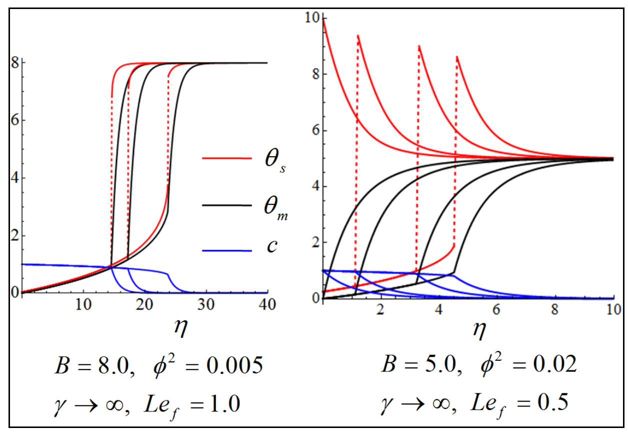

Figure2. Sample profiles of discontinuous solutions (or intermediate ignitions) between earliest and latest ignited solutions

Figure 2 shows the spatial profiles of average (or wall) temperature and concentration for two different parameter sets. The left and right most profiles correspond to earliest and latest ignited solutions while there can be infinite number of intermediate ignited solutions. Note the discontinuity in the average (or wall) temperature but not in the mixing-cup temperature or concentration. We also note that when $Le_f<1$ (figure 2b), the average (or wall) temperature may exceed the adiabatic temperature. Stability analysis (not shown here) indicated that each discontinuous solution is stable with a finite domain of initial conditions that are attracted to it.

Conclusions

We believe that our new results have profound implications that relate to the numerical solution of reacting flows, start-up and dynamic behavior of reactors and interpretation of experimental data. These will be discussed in the full manuscript.

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