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A Detection Algorithm for Bifurcations in Dynamical Systems using Reduced Order Models

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Abstract: Finite element or finite volume discretizations of distributed parameter systems (DPS) typically lead to high order finite dimensional systems. Model approximation is then an important first step towards the construction of optimal controllers. However, model reduction methods hardly take model uncertainties and parameter variations into account. As such, reduced order models are not well equipped when uncertain system parameters vary in time. This is particularly true when system behavior does not depend continuously on the parameters. It is shown in this paper that the performance of reduced order models inferred from Galerkin projections and proper orthogonal decompositions can deteriorate considerable when system parameters vary over bifurcation points. Motivated by these observations, we propose a detection mechanism based on reduced order models and proper orthogonal decompositions that allows to characterize the influence of parameter variations around a bifurcation value. for this, a hybrid model structure is proposed. The ideas are applied on the example of a tubular reactor. In particular, this paper discusses the difficulties in approximating the transition from extinction to ignited state in a tubular reactor.

1. INTRODUCTION

Many non-linear chemical processes show spatial-temporal characteristics which are usually modeled by means of distributed parameter systems (DPS). Finite element or finite volume techniques are commonly used to discretize a DPS so as to allow numerical simulations of DPS. Depending on the complexity and spatial geometry of the system, finite element approximations typically lead to high order approximations. The complexity of these models is often prohibitive when model based control system design or process optimization is the main purpose of the model. A common approach is to approximate the high order process by a simpler one, while keeping a sufficient level of accuracy. Various model reduction approaches are proposed in the literature. A particular popular method of model reduction is the technique of proper orthogonal decomposition (POD) (also known as the method Karhunen Loeve expansions). This method is widely used for obtaining reduced order models in computational fluid dynamics and has more recently been used for the approximation of chemical plants. A detailed analysis of POD-Galerkin projection is given in Holmes et al. [1996]. Its application for the identification of DPS systems is described in Zheng and Hoo [2002], while computer assisted studies towards control applications are given in Shvartsman and Kevrekidis [1998]. Some recent research is directed towards reducing DPS by using a gray box modeling approach Romijn et al. [2007] which showed significant computational savings. Some other interesting developments include multidimensional POD or tensorial POD van Belzen et al. [2007] which shows how low rank tensor approximations define suitable basis functions.

Most model reduction methods do not take model uncertainty or the effect of time-varying system parameters into account in the reduction process. The validity of reduced order models is then limited if the model is largely uncertain or if parameter variations lead to discontinuities in the process behavior. Indeed, if systems exhibit very drastic dynamical changes due to small parameter variations then this usually leads to a large mismatch between the system and its approximation. These kind of discontinuous dependence on system parameters is not at all uncommon in chemical engineering. Process parameters can show bifurcation or trifurcation phenomena of various types. For example, a jump from extinction to ignited states is the effect of a bifurcation value in well defined system parameter. Such effects are widely reported for many chemical processes. See, for example, some early work in

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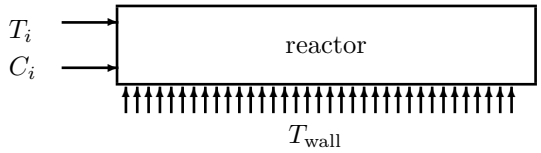

Fig. 1. Tubular reactor

Amundson [1970], Aris [1969], Hlavácek and Hoffmann [1970] that provide an analytical treatment to bifurcation phenomena. See also Jensen and Ray [1982].

This paper is motivated by the question on how to define reduced order models for systems that have uncertain time-varying parameters that exhibit strong discontinuities in dynamic responses. This question is of evident interest for questions on model validation. However, our prime motivation amounts to detecting, monitoring and controlling the parameters that cause abrupt changes in the system dynamics. For systems that exhibit bifurcation phenomena, we propose a hybrid model structure so as to allow a classification of system parameters around their bifurcation values.

Specifically, in this paper we consider a model of a tubular reactor where the Damkohler number is viewed as uncertain parameter that varies close to one of its bifurcation values. Changes of the Damkohler number correspond to the transition of the reactor from lower (extinction) to higher (ignited) states. Recently Bizon et al. [2007] studied the performance of reduced model of tubular reactor. In that paper, the tubular reactor was modeled as a chain of CSTR's. The performance of the reduced order model was studied as effect of inclusion of samples from a steady and an oscillatory regime.

In this paper we propose a simple detection mechanism on the basis of reduced order models. It processes the plant output and predicts the region of process operation (below or above a critical bifurcation parameter value).

This paper is organized by giving some background knowledge about existence of multiple steady state in chemical processes in section 2. Section 3 provides a brief summery on proper orthogonal decompositions. Section 4 proposes the detection mechanism while section 5 presents the results. Section 6 concludes the paper with some remarks on future research directions.

2. TUBULAR REACTOR MODEL AND MULTIPLE STEADY STATES

Considered a dynamical model of a tubular reactor as depicted in Figure 1.

The model represents a reactor with both diffusion and convection phenomena and a nonlinear heat generation term. The model is governed by the partial differential equations

$$\frac{\partial T}{\partial t} = \frac{1}{P_{\text{eh}}}\frac{\partial^2 T}{\partial z^2} - \frac{1}{L_e}\frac{\partial T}{\partial z} + \nu C e^{\gamma\left(1-\frac{1}{T}\right)} + \mu(T_{\text{wall}} - T) \tag{1a}$$

$$\frac{\partial C}{\partial t} = \frac{1}{P_{\text{em}}}\frac{\partial^2 C}{\partial z^2} - \frac{\partial C}{\partial z} - D_{\text{a}} C e^{\gamma\left(1-\frac{1}{T}\right)} \tag{1b}$$

which are subject to the mixed boundary conditions

$$\text{left side: } \begin{cases} \dfrac{\partial T}{\partial z} = P_{\text{eh}}(T - T_i) \\ \dfrac{\partial C}{\partial z} = P_{\text{em}}(C - C_i) \end{cases} \qquad \text{right side: } \begin{cases} \dfrac{\partial T}{\partial z} = 0 \\ \dfrac{\partial C}{\partial z} = 0 \end{cases}$$

See, e.g., Zheng and Hoo [2002]. $T(z,t)$ and $C(z,t)$ are dimensionless temperature and concentration variables, respectively, which are functions of time t and position z. Here, $t \in \mathbb{R}_+$ is the temporal independent variable and $z \in \Omega := [0,1]$ is the spatial independent variable. Inputs to the model are $u(t) = \text{col}(T_{\text{wall}}(t), T_{\text{i}}(t), C_{\text{i}}(t))$ which are the wall temperature, the inflow temperature and the inflow concentration, respectively. Initial conditions at time instant $t = 0$ are set to $T_0(z) = 1$ and $C_0(z) = 1$. The physical parameters of the system are mentioned in Jensen and Ray [1982] and given in the table below.

Peclet number (energy)	Peh	5
Peclet number (mass)	Pem	5
Lewis number	Le	1.0
Damkohler number	Da	bifur. para
Activation energy	γ	20.0
Adiabatic temperature rise	B	10.0
Heat of reaction	ν	0.8375
Heat transfer coefficient	μ	0

The model (1) is solved by the method of lines where the spatial domain $\Omega = [0,1]$ is gridded into 602 equidistant points. With the given initial and boundary condition, a time trajectory is simulated over 5000 time-samples of the state measurement (T, C).

Inputs of the model are

- Wall temperature $T_{\text{wall}}(t,z) = 1$ (dimensionless)
- Inflow conditions $T_i(t) = 1$, $C_i(t) = 1$
- Initial conditions $T_0(z) = 1$ and $C_0(z) = 1$.

Many tubular reactor models that occur in the literature can be adequately represented by this dimensionless model. The spatial gridding into 602 grid points is the result of a continued refinement of discretizations until the numerical solutions do not change further in accuracy. This is usually referred to as a converged Galerkin projection of an infinite dimensional system. Due to extremities in the process behavior under changes of the Damkohler number, numerical integrators easily fail to integrate the system state if the grid is too coarse. The model explains material and energy balances in the reactor. The PDEs (1) are parabolic in nature.

A classical analysis of tubular reactor model involves a lumping of the spatial coordinate and yields a model that is similar to a continuous stirred tank reactor (CSTR) model. In a CSTR, multiple steady states and oscillating solutions are observed as process parameter or process inputs such as inlet temperatures are changed. The balance between heat generation and heat removal defines the steady state at which the process is operating. A "lower steady state" (extinction) results when the reaction kinetics are limiting while "upper steady state" (ignition) shows heat exchange is limiting (limited cooling). Reactor shows a tendency to jump either to the upper or to the lower steady state.

Similar effects occur in the tubular reactor where transportation effects play a major role along with the reaction

and heat effects. The Damkohler number (Da) is the ratio of residence time to reaction time. Fast reactions have smaller reaction time and therefore large Damkohler numbers. For large Da values we have almost complete conversion. The Peclet number is the ratio of flow advection to flow diffusion. It is defined for mass and heat transfer. This number approaches infinity for plug flow reactors. For tubular reactors, the Peclet numbers larger than one. The Lewis number is the ratio of the physical transport thermal time constant to the physical transport material time constant. For a tubular reactor it is equal to one. Adiabatic temperature rise is the ratio of heat of reaction and average heat capacity of reactant and products. It is probably the most important parameter which determines the existence of multiple steady states. Highly exothermic reactions show increased chances of existence of multiple steady or periodic solutions. It is for this reason that bifurcation phenomena are usually studied in the Peclet-Da parameter space. For various values of the adiabatic temperature rise B, different parameter sets are obtained which may cause bifurcations of the solution set. The value $B = 10$ corresponds to the adiabatic case, where heating occurs at the reactor end (the hot spot). In turn, this increases the reaction rate at the reactor end, which further increases temperature. This effect persists and causes at a certain temperature and concentration, a jump from the lower to the higher steady state. Due to diffusion the larger concentration levels are carried throughout the reactor and lead to a higher steady state solution. The critical Damkohler value for which this jump of steady states occurs will be denoted by Da^*. Steady state solutions remain in the lower state for Damkohler values $\mathrm{Da} < \mathrm{Da}^*$ and lead to higher steady state values when $\mathrm{Da} > \mathrm{Da}^*$. More than sixteen different types of bifurcation structure have been reported in Jensen and Ray [1982]. Most of the literature on bifurcations in tubular reactors is devoted to finding conditions for existence of unique solutions, and to find the bounds over the parameter. Hlavácek and Hoffmann [1970] derived the bound $B < 4$ on the adiabatic temperature rise that guarantees uniqueness of solutions.

Stability analysis of the various chemical processes exhibiting multiple solutions has received large attention as well Jensen and Ray [1982], Shvartsman and Kevrekidis [1998], Hahn et al. [2004]. Eigenvalue analysis of the linearized system at resultant steady state is one of the easiest ways of stability estimation. Many times with Lyaponov functional, Poincare maps, phase diagram are employed to study it. Based on the eigenvalues two types of bifurcations are commonly reported. When real eigenvalues cross imaginary axis the resulting bifurcation is known as saddle node which result into bifurcation of stable solution when a pair of imaginary eigenvalues cross the imaginary axis we have Hopf bifurcation, which result into bifurcation of periodic solution.

3. PROPER ORTHOGONAL DECOMPOSITIONS

One of the most promising and significant techniques for an efficient reduction of large-scale nonlinear systems in fluid dynamics is the method of Proper Orthogonal Decompositions (POD) also known as the Karhunen-Loève method Holmes et al. [1996]. The method is based on the observation that flow characteristics reveal coherent structures or *patterns* in many processes in fluid dynamics. This has led to the idea that the solutions of model equations may be approximated by considering a small number of dominant coherent structures (called *modes*) that are inferred in an *empirical* manner from measurements or simulated data.

Given an ensemble of K measurements $\mathbf{T}^k(\cdot, t)$, $k = 1, \ldots, K$ with each measurement defined on some spatial domain Ω, the POD method amounts to assuming that each observation $\mathbf{T}^k$ belongs to a Hilbert space $\mathcal{H}$ of functions defined on Ω. With the inner product defined on $\mathcal{H}$, it then makes sense to call a collection $\{\varphi_j\}_{j=1}^{\infty}$ an *orthonormal basis* of $\mathcal{H}$ if any element, say $\mathbf{T} \in \mathcal{H}$, admits a representation

$$\mathbf{T}(x) = \sum_{j=1}^{\infty} a_j \varphi_j(x), \quad x \in \Omega.$$

Here, the a_j's are referred to as the *coefficients* and the φ_j's are the *modes* of the expansion. The truncated expansion

$$\mathbf{T}_n(x) = \sum_{j=1}^{n} a_j \varphi_j(x), \quad x \in \Omega$$

causes an approximation error $\|\mathbf{T} - \mathbf{T}_n\|$ in the norm of the Hilbert space. We will call $\{\varphi_j\}_{j=1}^{\infty}$ a *POD basis* of $\mathcal{H}$ whenever it is an orthonormal basis of $\mathcal{H}$ for which the *total approximation error* $\sum_{k=1}^{K} \|\mathbf{T}^k - \mathbf{T}_n^k\|$ is minimal for all truncation levels n. This is an *empirical basis* in the sense that every POD basis depends on the data ensemble.

Using variational calculus, the solution to this optimization problem amounts to finding the normalized eigenfunctions $\varphi_j \in \mathcal{H}$ of a positive semi-definite operator $R : \mathcal{H} \to \mathcal{H}$ that is defined as

$$\langle \psi_1, R\psi_2 \rangle := \frac{1}{K} \sum_{k=1}^{K} \langle \psi_1, \mathbf{T}^k \rangle \cdot \langle \psi_2, \mathbf{T}^k \rangle$$

with $\psi_1, \psi_2 \in \mathcal{H}$. R is well defined in this manner and corresponds to a positive semi-definite matrix whenever $\mathcal{H}$ is finite dimensional. In that case, a POD basis is obtained from the normalized eigenvectors of R Astrid [2004].

Subsequently, a Galerkin projection is used to obtain the reduced model as follows. Suppose that the system is governed by a PDE of the form

$$\frac{\partial T_n}{\partial t} = \mathcal{A}(T_n) + \mathcal{B}(u) + \mathcal{F}(T_n, u, d) \tag{2}$$

Let $\mathcal{H}_n$ denote an n dimensional subspace of $\mathcal{H}$ and let $P_n : \mathcal{H} \to \mathcal{H}_n$ and $I_n : \mathcal{H}_n \to \mathcal{H}$ denote the canonical projection and canonical injection maps. The reduced model is then given by

$$P_n \frac{\partial T_n}{\partial t} = P_n \mathcal{A}(T_n) + P_n \mathcal{B}(u) + P_n \mathcal{F}(T_n, u, d) \tag{3}$$

where $T_n(\cdot, t) = \mathbf{T}_n(t)$ belongs to $\mathcal{H}_n = P_n \mathcal{H}$ for all t. In the specific case of a POD basis, the finite dimensional subspace $\mathcal{H}_n = \mathrm{span}(\varphi_1, \ldots, \varphi_n)$ where the φ_j's denote POD basis functions. In that case, (3) becomes an *ordinary differential equation* in the coefficients $a_j(t)$ in the expansion of T_n.

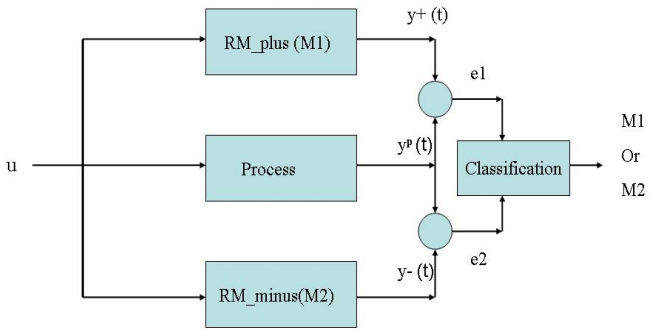

Fig. 2. Dynamic error detection mechanism.

4. METHODOLOGY

Schematic idea of proposed methodology is shown in Figure 2. The motivation for this methodology comes from the fact that process has two different kinds of limitation in bifurcation range - before and after bifurcation. For bifurcation parameter (which is Damkohler number in our example) below critical bifurcation value - reaction rate is limiting while above the critical value heat exchange is limiting. This result into two completely different reactor behavior which is highly difficult to capture into single reduced model. The difficulty arises due to the limitation imposed by POD which is good for the system behavior it has been trained for by including such dominant pattern in the snapshots. Based on the bifurcation parameter value below or above critical ($Da^- < Da^* < Da^+$) systems will behave differently. Such system exhibiting two extreme behavior can be approximated by knowing in which regime process is operating in. If process is operating for parameter below critical bifurcation value then it will be approximated by reduced model RM_minus else by RM_plus. The reason for not including the transition from lower to higher steady state and other details are explained in the result section.

5. RESULTS AND DISCUSSION

5.1 Bifurcation study on full model

The PDEs governing the tubular reactor model are descritized by the method of lines so as to represent the model as a finite number of differential equations. The discretized system is of state dimension $n = 602$. This system is simulated for Damkohler numbers $\mathrm{Da} < \mathrm{Da}^*$ and $\mathrm{Da} > \mathrm{Da}^*$ below and above the bifurcation value Da^*. Figure 3 shows the dynamic response of the tubular reactor for these values.

Initial conditions for temperature and concentration were equal to unity, while all system input mentioned in section 3 were constant and equal to 1. Left side plots are before bifurcation and right side are after bifurcation. Upper plots show temperature and lower plots show concentration. Time, reactor length and both variables are in dimensionless form.

The simulation results in Figure 3 show that for the given parameter values, the bifurcation parameter range

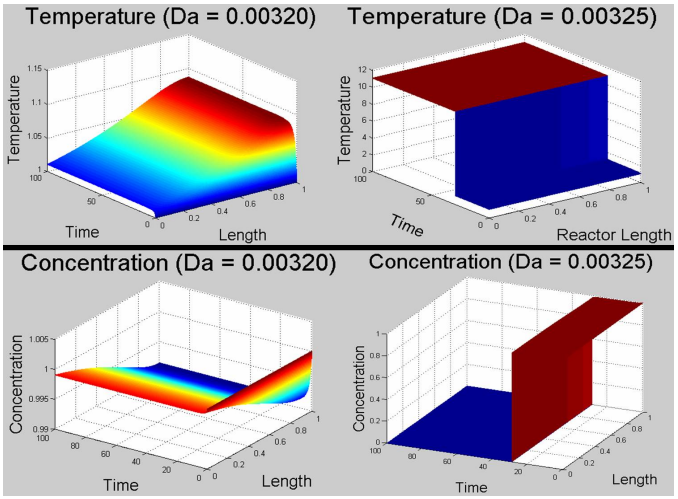

Fig. 3. Behavior of tubular reactor before and after bifurcation.

($Da^- < Da^* < Da^+$) is ($0.00320 < Da^* < 0.00325$). This means that for certain Da^* there exist multiple steady states. It also means that for all simulations of adiabatic reactor ($\mu = 0$) with Damkohler number $\mathrm{Da} < \mathrm{Da}^- = 0.00320$ the system shows lower steady state which is characterized by slow reaction and lower temperature rise. As the reactor is adiabatic in nature, we see the location of the hot-spot at the reactor end. For $Da^+ > 0.00325$, the system jumps from lower to higher steady state. Around $\mathrm{Da} = 0.03000$, an immediate jump occurs from the initial condition. In Jensen and Ray [1982], three steady states are reported for these parameter ranges. However, it is difficult to observe the middle steady state by dynamic simulations. This middle steady state is usually said to be unstable. By using software Doedel et al. [1997] one can find this middle state as well. Operating at this middle state could be optimal sometimes.

5.2 Model reduction

Model reduction for the given system is explained into 3 parts: For Damkohler numbers $Da < Da^*$, for values ($Da^* \leq Da < Da_2^+$) and for upper range of Da^+ ($Da \geq Da_2^+$) which shows an immediate jump of steady state solutions. As all three parameter ranges result into different spatial profiles, it is difficult to capture all three behaviors by one reduced model that is inferred from a Galerkin-POD reduction method. But it is still very attractive that we are classifying the parameter space in these three regions. It will be shown that a partition of the parameter space in these three regions is enough to consider whole Da space, assuming that other process parameter are constant.

MR and Detection Mechanism for $Da < Da^*$ and for $Da \geq Da_2^+$ This range of Da gives either lower or higher steady state. It means we can lump all possible Da values in either group Da^- or in group Da^+. Galerkin-POD method is known for its sensitivity to any other perturbation than it is trained for. It means if we get snapshot for certain combination of input, initial condition, parameter values, then obtained basis function will not be able to represent the system dynamics for other combination of

parameters. This happens due to spatial directionality that is inherent to the basis functions. Sometimes a simple trick is used, to combine in time the snapshots of different perturbation; performing POD over such snapshot will then give (common) basis function which will have good performance for all the complete parameters range. But one should not try to get common basis for extreme parameters as then obtained basis will not perform well for either of the parameters. To get these common basis function one simply stack up the snapshots that are obtained for certain parameter range. One must stack them up in time if one is interested in getting spatial basis. We tried to get common basis functions in similar way for $Da < Da^*$ (i.e. to approximate lower steady state by POD) and for Da values quite large ($Da > Da_2^+$) such that system jumps from initial condition immediately (i.e. to approximate higher steady state) . The basis obtained for former ($Da^- < Da^*$) hence works good to approximate original systems with Da less than bifurcation value. Similar holds for $Da > Da_2^+$. Figure 4 shows the same thing, that error (static error - normed over space and time) in reconstruction of snapshot for various values of Da before and after bifurcation. Figure also shows that common basis obtained by Da^- gives small error in reconstruction of snapshots for values of Da in Da^- space where as they give large error when we try to reconstruct the snapshots of Da^+. Similar results are obtained when we use common basis of $Da > Da_2^+$.

If $\Phi = \text{span}(\varphi_1, \ldots, \varphi_n)$, denotes POD basis functions which span the subspace $\mathcal{H}_n$ as given in section(3) then static error of snapshot reconstruction can be given by

$\varepsilon = (I - \Phi * \Phi') * \mathbf{T}^k(\cdot, t)$ where $\mathbf{T}^k(\cdot, t)$ is an ensemble (snapshot matrix) of K measurements $k = 1, \ldots, K$

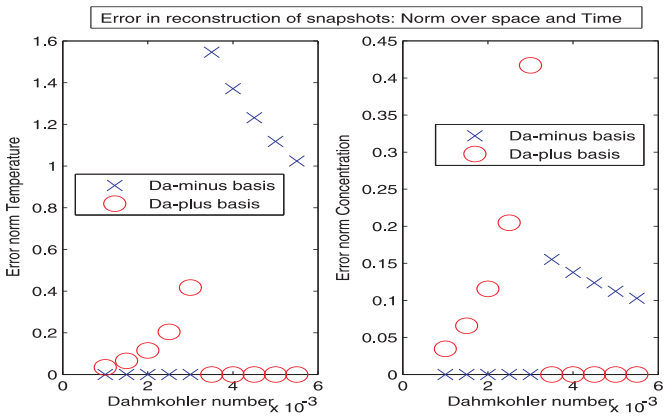

Fig. 4. Results of static error detection mechanism.

This can be said as *static detection mechanism* to detect bifurcation. Given snapshot data for any Da value by finding the static error of snapshot reconstruction by using common basis of Da^+ and Da^- one can find out the operation regime of the process. Basis functions which gives minimum error is the one where process is most likely to be operating in, and one can use corresponding reduced model. Dynamic error detection mechanism as given in methodology section can then be applied which will approximate full scale model by either of the reduced model based on error criteria of dynamic detection mechanism. Figure 5 shows temperature and concentration at the middle of the reactor of full model which jumps from lower state to higher as Da changes from Da^- to Da^+ and two reduced models. At any instant, either of the reduced models shows behavior close to the full model. Model which gives minimum error (spatial norm) is the one which can be selected. Each of the reduced model needs around 3-4 basis functions which captures $\sim 99\%$ of the energy.

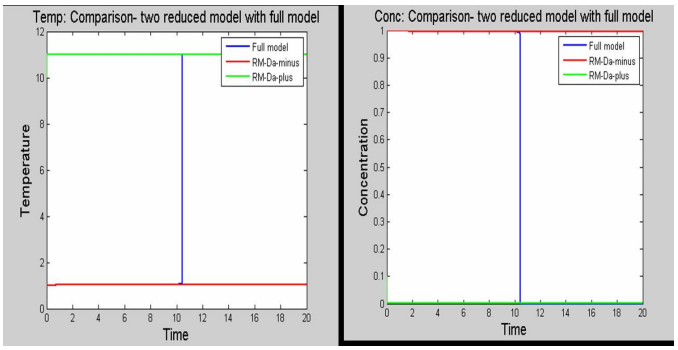

Fig. 5. Comparison of full scale and two reduced models of tubular reactor

MR for $Da \geq Da^*$ and for $Da < Da_2^+$ In this range of Da, we see transition from lower to higher state as a dynamic effect. This is the most interesting case as if one is able to capture this transition in efficient reduced model then there is no need to have the detection mechanism as mentioned in methodology section. But it is not possible to approximate this model by a reduced one by using few basis functions. The reason is that, while transition the full scale model shows spatio-temporal phenomenon called 'traveling waves'. This is seen due to the inherent diffusive nature of tubular reactor model. More on traveling wave can be founding Marquardt [1990]. In the first bit of this section it was mentioned that due to adiabatic nature of the reactor hot spot is located at reactor end. During jump from lower to higher state, reactor end is the first point which shows this jump and then due to diffusions, the next point jumps and in that fashion whole reactor jumps to ignited state. As this jump is initiated from reactor end (right side) we see a wave traveling through the reactor from right to left side of the reactor. When one observes it in time, it is seen that the wave travels very fast (compared to residence time of reactants in the reactor) such that it seems the whole reactor is ignited at one instant. It is difficult to capture the wave pattern by using POD due to the resultant triangular snapshot matrix. When snapshot matrix is of such form the common notion of capturing $\sim 99\%$ energy in few basis functions is not possible and one must use high order reduced model which computationally are not attractive. Figure 6 shows the wave pattern of temperature and concentration in the reactor during the transition.

6. CONCLUSIONS

In this paper we presented a new methodology to approximate a model of a parameter varying tubular reactor by a hybrid model structure that consists of two reduced order models. The parameter variation was chosen so as to exhibit a discontinuous dependence of the dynamical

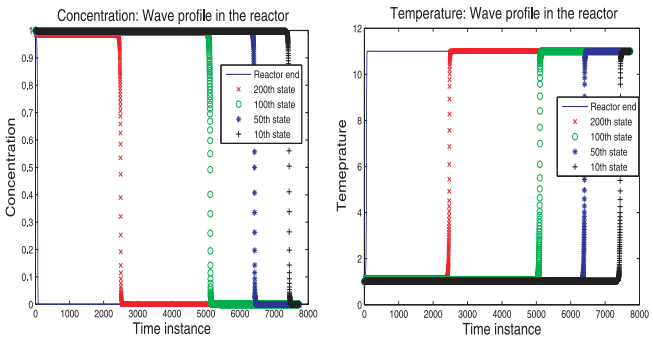

Fig. 6. Wave pattern in the reactor

responses as function of the parameter (the Damkohler number in the reaction). A critical value of the Damkohler number causes the steady state response of the system to change from a lower to a higher value. We presented both a static and dynamic detection mechanism for which it is easy to detect whether the parameter value is below or above a critical value. In an on-line fashion the algorithm allows to detect the parameter regime in which the process is running. An investigation of the corresponding wave patterns in the reaction shows the difficulty to capture the transition from lower to higher state in the reduced model.

Future work includes- application of devised methodology on industrial glass manufacturing process, investigation to capture wave pattern, optimal sensor placement problem based on missing point estimation to detect bifurcation in advance to help control action, observer design problem, computational aspects, exploiting the knowledge of bifurcation phenomena for optimal process design and controller tuning aspects, and possibility of employing temporal basis function.

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