ACCELERATED KARHUNEN LOÈVE EXPANSION APPLIED TO MODEL REDUCTION

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Abstract: The distributed behavior of a chemical system can be represented by a system of partial differential equations. The general solution of this representation gives rise to a high order system with infinite dynamics which cannot be used for an application such as control. Given an exact model of the system, this work discusses the use of *accelerated* empirical eigenfunctions as basis functions in a nonlinear Galerkin method to arrive at a reduced-order solution. The technique is applied to the hydro-dealkylation of toluene and the quality of the results are compared to those obtained using standard Galerkin method.

Keywords: Moment methods, Reduced-order models, Nonlinear systems

1. INTRODUCTION

A large number of chemical processes can be described accurately by a system of partial differential equations (PDEs) in which the independent variables are one or more spatial variables and time. Examples include, the heat equation and the kinematic wave equation. Solutions of these systems are infinite series solutions that meet certain boundary conditions based on the problem to be solved. To use these solutions in an application such as control will require suitable discretizations of the governing equations. Such discretizations are computationally expensive and also cumbersome to work with (Zheng, 2003).

One approach to obtain low order models is based on the existence of an Inertial Manifold (IM). The existence of an IM for a class of nonlinear dissipative PDEs was confirmed by (Foias *et al.*, 1989). On an IM, all the trajectories of the long time behavior decay exponentially to a *global attractor*. The dissipative nature of the long time behavior of the system means that the behavior can be characterized by a small number of active degrees of freedom. The fact that for many classes of dissipative dynamical systems there exists an IM is significant because properties such as stability can be analyzed by a study of the inertial form (ordinary differential equation on the IM). The interested reader is referred to the work of (Shvartsman and Kevrekidis, 1998). When an explicit form of the IM cannot be derived, an approximate inertial manifold (AIM) can be generated by successive substitution (Zheng, 2003). The criteria for existence of an AIM were presented for nonlinear parabolic evolution equations by (You, 1995).

Another approach to obtain low order models is based on a statistical analysis of the spatio-

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temporal data obtained from the system (Holmes *et al.*, 1996; Sirovich *et al.*, 1990). A semi-empirical method such as Proper Orthogonal Decomposition or the Karhunen-Loève expansion (KL) is applied to the data which yields a set of empirical eigenfunctions (EEFs). These EEFs are combined with a standard PDE solution approach such as the Galerkin method to transform the original infinite-order system into one with finite-order dynamics while retaining the long time behavior. The method has been widely applied in a variety of fields ranging from hydrodynamics (Holmes *et al.*, 1996) to reaction engineering (Zheng and Hoo, 2002*b*).

While these methods have been successful with a large number of problems, for certain systems the solution may not be accurate. For instance, in a study by (Sirovich *et al.*, 1990) of the complex Ginzburg-Landau equation, it was shown that a standard KL-Galerkin solution was less accurate (based on the Lyapunov dimension) when Dirichlet boundary conditions were applied. Similar observations were found by (Zheng, 2003) when a standard KL-Galerkin method was used to develop a reduced-order model of a nonlinear tubular reactor system. This lack of accuracy will impact important applications such as model-based control and monitoring that require low order models for implementation reasons. Thus, the objective of developing accurate reduced-order models for these types of applications provides the motivation for considering an alternate approach.

In this work, an approach that retains some of the modes that are excluded in the identification of the EEFs is examined (Sirovich *et al.*, 1990). These new EEFs are called *accelerated* EEFs (aEEFs) and when applied with the Galerkin method they produce a nonlinear Galerkin solution. This approach differs from the AIM method because the solution found from the latter assumes pseudo-steady state of the fast modes. In the determination of the aEEFs, the time derivative of the data is used. This difference provides insights into how the system changes with time as long as the data themselves are of high fidelity.

The paper is organized as follows: Section 2 develops the accelerated nonlinear KL-Galerkin method. Section 3 demonstrates the approach on a nonlinear tubular reactor system and compares the results to the solution obtained using a standard (linear) KL-Galerkin method. The final section contains concluding remarks.

2. METHODOLOGY

2.1 Standard Karhunen-Loève Expansion

The Karhunen-Loève expansion is a linear procedure that generates basis functions that correspond to the dominant modes of the dynamical system. These basis functions are the *empirical eigenfunctions* (EEFs) (Holmes *et al.*, 1996; Sirovich *et al.*, 1987) of the system. If the system is dissipative, then the long time behavior can be characterized by a small number of degrees of freedom. Thus, only a small number of EEFs are necessary to describe the system resulting in a reduction in the order of the model without loss of complexity (Newman, 1996). The procedure employed to generate the EEFs uses data taken from the system. The procedure is summarized as follows (Sirovich *et al.*, 1987):

1 Data are collected at different spatial points at regularly spaced time intervals. These data may be plant data or simulated data taken from a mathematical description of the plant. In either case, the data represent perturbations about a nominal state. It is important that the data contain information about the dynamic behavior of the system and are of high fidelity.
2 A set of data points at any given time is called a *snapshot* of the system at that time. The data are arranged as an ensemble of snapshots. It is assumed that the ensemble has a single average.
3 The spatial correlation matrix of the snapshots is calculated. Under the assumption of *ergodicity* (Newman, 1996), the spatial correlation matrix defines an eigenfunction / eigenvector problem whose eigenfunctions are the empirical eigenfunctions of the system.

It has been shown that the EEFs are optimal in the sense of the energy captured from the data. The first few EEFs capture most of the energy of the system where the largest EEFs correspond to the slowly evolving modes of the system. If for some systems the eigenspectrum is not separated, then a large number of EEFs may be necessary to capture greater than 90% of the energy in the system. One such system has been discussed by (Zheng and Hoo, 2002*b*).

2.2 Accelerated Karhunen-Loève Expansion

The basic concept of generating *accelerated* EEFs is to use the information from the time derivative of the data to capture the nonlinearity of the system. The following description is adapted from the work of (Sirovich *et al.*, 1990) and (Zheng, 2003). Consider the PDE given by,

$$\begin{aligned} \frac{\partial \mathbf{x}}{\partial t} &= \dot{\mathbf{x}}(z,t) = \mathcal{A}\mathbf{x}(z,t) = f(\mathbf{x}) \\ \mathcal{A} &= \alpha \frac{\partial^2}{\partial z^2} - \nu \frac{\partial}{\partial z} \end{aligned} \tag{1}$$

where $\alpha, \nu > 0$, $z \in \Omega \subset R$, $t \geq 0$, and $\mathbf{x} \in R^n$. By the Karhunen-Loève theorem, for the differential system given in (1),

$$\dot{\mathbf{x}}(z,t) = \sum_{k=1}^{\infty} \langle \psi_k, \dot{\mathbf{x}} \rangle \psi_k = \sum_{k=1}^{\infty} b_k(t) \psi_k(z) \tag{2}$$

where the set $\{\psi\}$ is a complete orthonormal basis set in the function space and $\langle \cdot, \cdot \rangle$ denotes an inner product under which $\{\psi\}$ is orthonormal. The coefficients $\{b_k\}$ are the projections of $\dot{\mathbf{x}}$ onto the functions $\{\psi\}$.

Let $\mathcal{P}_N$ be the projection operator onto the first N elements of $\{\psi\}$ and $\bar{\psi}_N \equiv \{\psi_1, .., \psi_N\}$. Such an operator will give a finite truncation, $\dot{\mathbf{x}}_N$, of $\dot{\mathbf{x}}$. Let $\mathcal{Q}_C$ be the complement of $\mathcal{P}_N$ such that $\mathcal{Q}_C \equiv (1 - \mathcal{P}_N)$. Applying the projection operators to the system in (1) and using (2) gives,

$$\begin{aligned} \mathcal{P}_N \dot{\mathbf{x}} &= \dot{\mathbf{x}}_N = \langle \bar{\psi}_N, \dot{\mathbf{x}} \rangle = \sum_{k=1}^{\infty} \langle \bar{\psi}_N, \psi_k \rangle b_k(t) \\ \mathcal{Q}_C \dot{\mathbf{x}} &= \dot{\mathbf{x}}_C = \langle \bar{\psi}_C, \dot{\mathbf{x}} \rangle = \sum_{k=1}^{\infty} \langle \bar{\psi}_C, \psi_k \rangle b_k(t) \\ \dot{\mathbf{x}} &= \dot{\mathbf{x}}_N + \dot{\mathbf{x}}_C \end{aligned} \tag{3}$$

and $\bar{\psi}_C \equiv \{\psi_{N+1}, .., \psi_\infty\}$. With respect to the right hand side of (1),

$$\begin{aligned} \dot{\mathbf{x}}_N &= \mathcal{P}_N f(\mathbf{x}) = \mathtt{F}(\mathbf{x}_N + \mathbf{x}_C) \\ \dot{\mathbf{x}}_C &= \mathcal{Q}_C f(\mathbf{x}) = \mathtt{R}(\mathbf{x}_N + \mathbf{x}_C). \end{aligned} \tag{4}$$

The slow modes of the system are represented by $\mathbf{x}_N$ and the fast modes by $\mathbf{x}_C$. The slow modes evolve slowly in time and hence dominate the long time behavior of the system. In the standard Galerkin procedure, $\mathbf{x}_C = 0$ such that $\dot{\mathbf{x}}_N = \mathtt{F}(\mathbf{x}_N)$ and $\mathtt{R}(\mathbf{x}_N) = 0$.

Suppose the set $\{\psi\}$ is selected such that $\mathtt{R}$ is minimized, i.e. $\|\mathtt{R}\|$. Then, $\mathtt{R}(\mathbf{x}_N + \mathbf{x}_C) = 0$ implying that the fast modes can be made a function of the slow ones. This approach is similar to the AIM method, however in the AIM approach, the fast modes are necessarily functions of the slow modes because of the pseudo-steady state assumption of the fast modes.

The minimization of $\mathtt{R}$ implies a minimization of $\|\dot{\mathbf{x}}_C\|^2 (< \epsilon)$ or a maximization of $\|\dot{\mathbf{x}}_N\|^2$. These quantities are time dependent. Thus, the ensemble time average given by

$$\dot{E} = (\langle \dot{\mathbf{x}}_N, \dot{\mathbf{x}}_N \rangle) \tag{5}$$

is maximized.

Let $\{\dot{\mathbf{x}}(z, t_n)\} \equiv \{\dot{\mathbf{x}}^{(n)}\}$, be an ensemble ($M$ members) of uniform samples of the states in (1). The spatial correlation function of this process is given by,

$$L(z,\zeta) = \lim_{M \to \infty} \frac{1}{M} \sum_{n=1}^{M} \dot{x}_i^{(n)} \dot{x}_j^{(n)}.$$

By Mercer's theorem,

$$L(z,\zeta) = \sum_{k=1}^{\infty} \lambda_k \psi_k(z) \psi_k(\zeta) \tag{6}$$

where $\{\lambda_k\}$ are the eigenvalues and $\{\psi_k\}$ are the *accelerated* eigenfunctions of $L(z,\zeta)$. The infinite series in (6) converges absolutely and uniformly on $\Omega \times \Omega$. It then follows that (Ash and Gardner, 1975)

$$\int_\Omega L(z,\zeta) \psi_j(\zeta) d\zeta = \lambda_j \psi_j(z).$$

The above result also implies that the set $\{\psi\}$ can be obtained from the data ($\dot{\mathbf{x}}$).

Since the operator $\mathcal{P}_N$ serves to produce a finite truncation, then $\dot{\mathbf{x}}_N$ can be associated with the coefficients $\mathbf{b}_N = \{b_k(t)\}_{k=1}^N$. Similarly, $\dot{\mathbf{x}}_C$ is associated with $\mathbf{b}_C$ and $\{\mathbf{b}\} = \{\mathbf{b}_N + \mathbf{b}_C\}$.

The following dynamical system can be formulated,

$$\begin{aligned} \frac{d\dot{\mathbf{x}}}{dt} &= \sum \frac{db_k}{dt} \psi_k = \frac{d}{dt} f(\mathbf{x}) \\ \mathcal{P}_N \frac{d\dot{\mathbf{x}}}{dt} &= \frac{d\mathbf{b}_N}{dt} = \mathtt{S}_N(\mathbf{b}_N, \mathbf{b}_C) \\ \mathcal{Q}_C \frac{d\dot{\mathbf{x}}}{dt} &= \frac{d\mathbf{b}_C}{dt} = \mathtt{S}_C(\mathbf{b}_N, \mathbf{b}_C). \end{aligned} \tag{7}$$

The maximization of (5) implies

$$(\|\dot{\mathbf{b}}_C\|) < \epsilon.$$

Therefore, the above dynamical system in (7) becomes

$$\begin{aligned} \frac{d\mathbf{b}_N}{dt} &= \mathtt{S}_N(\mathbf{b}_N, \mathbf{b}_C) \\ 0 &= \mathtt{S}_C(\mathbf{b}_N, \mathbf{b}_C). \end{aligned} \tag{8}$$

It is noted that the deliberate requirement by (5) led to the system in (8). The algebraic part of the above system can be solved readily for $\mathbf{b}_C$ as a function of $\mathbf{b}_N$.

3. HDA PROCESS

The hydro-dealkylation (HDA) of toluene to produce benzene has been studied extensively in the open literature. The following description is taken from (Zheng, 2003). The known reactions are,

$$\begin{aligned} R_1 &: \quad C_7H_8 + H_2 \rightarrow C_6H_6 + CH_4 \\ R_2 &: \quad 2C_6H_6 \rightleftharpoons C_{12}H_{10} + H_2 \end{aligned} \tag{9}$$

The process flowsheet has two feed streams: a pure liquid toluene stream at ambient conditions, and a gaseous hydrogen stream consisting of 95 mole percent hydrogen and 5 mole percent methane, at 100^oF and 560 psia. The objective of the design is to produce benzene at a rate of 256 lbmole/hr and at a purity of 99.7%.

The reactor operating pressure is 500 psia, and to realize a satisfactory reaction rate, the inlet reactor temperature should be above 1150^oF, but the reactor temperature itself should not exceed 1300^oF to prevent hydrocracking. Further, the hydrogen-toluene feed ratio at the reactor inlet should be at five to one or larger to reduce coking and to reduce product loses by R_2. Also, the reactor effluent stream must be quenched rapidly to at least 1150^oF to prevent coking in the heat exchanger that follows the reactor.

The process in the tubular reactor can be described by the following system of nonlinear, dimensionless PDEs,

$$\frac{\partial \xi_1}{\partial \tau} = -\nu \left[\frac{\partial \xi_1}{\partial \tau_1} + \frac{\xi_1}{\theta} \frac{\partial \theta}{\partial \tau_1} \right] - \xi_1 \xi_2^{0.5} \theta^{1.5} \mathrm{e}^{\gamma_1 \frac{\theta - 1}{\theta}}$$

$$\frac{\partial \xi_2}{\partial \tau} = -\nu \left[\frac{\partial \xi_2}{\partial \tau_1} + \frac{\xi_2}{\theta} \frac{\partial \theta}{\partial \tau_1} \right] - \xi_1 \xi_2^{0.5} \theta^{1.5} \mathrm{e}^{\gamma_1 \frac{\theta - 1}{\theta}} + \kappa_2 (\xi_3 \theta)^2 \mathrm{e}^{\gamma_2 \frac{\theta - 1}{\theta}} - \kappa_3 \xi_2 \xi_5 \theta^2 \mathrm{e}^{\gamma_3 \frac{\theta - 1}{\theta}}$$

$$\frac{\partial \xi_3}{\partial \tau} = -\nu \left[\frac{\partial x_3}{\partial \tau_1} + \frac{\xi_3}{\theta} \frac{\partial \theta}{\partial \tau_1} \right] + \xi_1 \xi_2^{0.5} \theta^{1.5} \mathrm{e}^{\gamma_1 \frac{\theta - 1}{\theta}} - 2\kappa_2 (\xi_3 \theta)^2 \mathrm{e}^{\gamma_2 \frac{\theta - 1}{\theta}} + 2\kappa_3 \xi_2 \xi_5 \theta^2 \mathrm{e}^{\gamma_3 \frac{\theta - 1}{\theta}}$$

$$\frac{\partial \xi_4}{\partial \tau} = -\nu \left[\frac{\partial \xi_4}{\partial \tau_1} + \frac{\xi_4}{\theta} \frac{\partial \theta}{\partial \tau_1} \right] + \xi_1 \xi_2^{0.5} \theta^{1.5} \mathrm{e}^{\gamma_1 \frac{\theta - 1}{\theta}}$$

$$\frac{\partial \xi_5}{\partial \tau} = -\nu \left[\frac{\partial \xi_5}{\partial \tau_1} + \frac{\xi_5}{\theta} \frac{\partial \theta}{\partial \tau_1} \right] + \kappa_2 (\xi_3 \theta)^2 \mathrm{e}^{\gamma_2 \frac{\theta - 1}{\theta}} - \kappa_3 \xi_2 \xi_5 \theta^2 \mathrm{e}^{\gamma_3 \frac{\theta - 1}{\theta}}$$

$$\frac{\partial \theta}{\partial \tau} = \frac{1}{\zeta} \left[H_{r_1} \frac{\partial \xi_1}{\partial \tau} - H_{r_2} \frac{\partial \xi_5}{\partial \tau} + Q(\theta_F - \theta) - \nu \left(\zeta \frac{\partial \theta}{\partial \tau_1} - H_{r_1} \frac{\partial \xi_1}{\partial \tau_1} + H_{r_2} \frac{\partial \xi_5}{\partial \tau_1} \right) - F_{Bm} \zeta_B \right]$$

$$z = 0 \qquad \begin{cases} \xi_j = \xi_j(t = 0) \quad j = 1, \ldots, 5 \\ \theta = \theta(t = 0) \end{cases}$$

$$z = 1 \qquad \begin{cases} \dfrac{\partial \xi_j}{\partial z} = 0 \quad j = 1, \ldots, 5 \\ \dfrac{\partial \theta}{\partial z} = 0 \quad . \end{cases}$$

where $\xi_j, j = 1 \ldots 5$ represents the concentrations of toluene, hydrogen, benzene, methane, and diphenyl, respectively; θ represents the temperature; and $\tau = t/t_{cr}$ is the dimensionless time. The initial feed compositions of toluene, hydrogen, and methane are {0.0807, 0.4035, 0.5158}, respectively. See Table 1 for other values.

Table 1. Table of parameter Values

Parameter	Nominal Values
F_{bm}	0.0
$\theta_F = \dfrac{T_F}{T_0}$	1.0
$t_{cr} = \dfrac{C_0}{k_1(T_0) P_0^{3/2}}$	2.077
$k_1(T_0)$	1.0
$\kappa_2 = \dfrac{k_2(T_0) P_0^2}{k_1(T_0) P_0^{1.5}}$	0.995
$\kappa_3 = \dfrac{k_3(T_0) P_0^2}{k_1(T_0) P_0^{1.5}}$	5.34
$H_{R_1} = \dfrac{H_{R_1}}{\hat{c}_{p0} T_0}$	-1.51
$H_{R_2} = \dfrac{H_{R_2}}{\hat{c}_{p0} T_0}$	-0.473
$Q = \dfrac{u(s/v) t_{cr}}{\hat{c}_{p0} T_0 C_0}$	0.0
$\gamma_1 = \dfrac{E_a}{R T_0}$	29.26
$\gamma_2 = \dfrac{E_a}{R T_0}$	29.68
$\gamma_3 = \dfrac{E_a}{R T_0}$	33.49

3.1 Results

The system of PDEs describing the HDA process is solved using the method of finite differences (FD) with 101 spatial points. This solution is considered the true solution. Simulated data (snapshots) are taken from the FD solution to determine the EEFs and the aEEFs where it is assumed that there are five temperature sensors located along the tubular reactor (z=0, 1/3, 1/2, 2/3, 1), but all composition measurements are available only at the exit (z=1) of the reactor. The data are collected over a range of $0 < F_{Bm} < 0.003$ and a ±2% change in the reactor pressure. Figure 1 shows the first two EEFs found for each of the methods (linear KL:△, ▽ and aKL:○, ●) for the temperature data. Table 2 shows the associated eigenvalues of the temperature and benzene data. The first three eigenvalues capture >95% of the energy in the data.

In order to find the best reduced-order models, two and three EEF (mode) models for both temperature and benzene are examined, in the linear KL-Galerkin case. These models are tested in the presence of 3% increase in reactor pressure and 0.15% increase in benzene injection flowrate

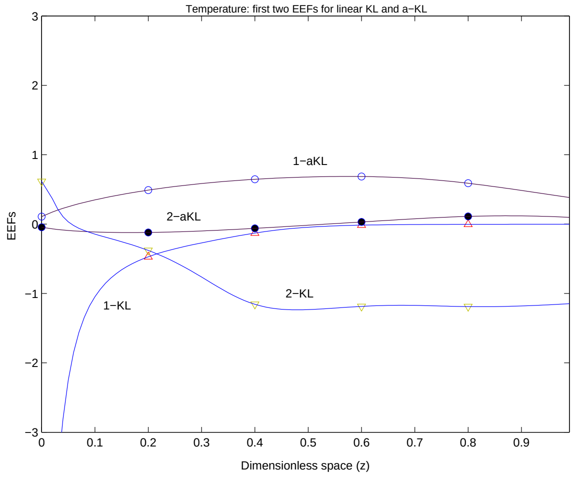

Fig. 1. Eigenfunctions of the temperature data.

Table 2. The first 3 eigenvalues.

Eigenvalues	Temperature		Benzene	
	KL	aKL	KL	aKL
1	0.9814	0.9922	0.9827	0.7220
2	0.0125	0.0066	0.0056	0.2108
3	0.0043	0.0008	0.0006	0.0290
Cum	0.9882	0.9996	0.9889	0.9618

(F_{Bm}). Using the Integral of the Time Averaged Error (ITAE) as a measure of fit to the data, it is found that the two-EEF models (second order) give the smallest error.

Since the development of the aKL models considers the fast modes only as functions of the slow modes, the order of the model is equal to the number of slow modes used. The ITAE measure in the aKL case indicates that for temperature, a second order model, with the third and fourth modes expressed as functions of the first two, is the best. Similarly for benzene, a first order model with one slow and two fast modes gave the lowest ITAE.

The ITAEs for the best models are given in Table 3.

Table 3. ITAE for the best models.

	Temperature		Benzene	
	KL	aKL	KL	aKL
Nominal	0.0066	0.0049	0.0093	0.0024
3%inc Pres	0.7182	0.5116	0.3693	0.1553
0.15% F_{Bm}	0.8629	0.7001	1.0311	0.9315

Figure 2 compares the results of the reduced-order models used in the KL-Galerkin (△) and aKL-Galerkin (○) methods to that of the FD (◇) solution at the nominal conditions. Figures 3 and 4 show the model fit of temperature and benzene for a 3% increase in the reactor pressure and a 0.15% increase in F_{Bm}, respectively. The aKL models fit the dynamics better than the KL models in both the temperature and benzene responses. Higher order KL models (not shown) did not improve the overall fit.

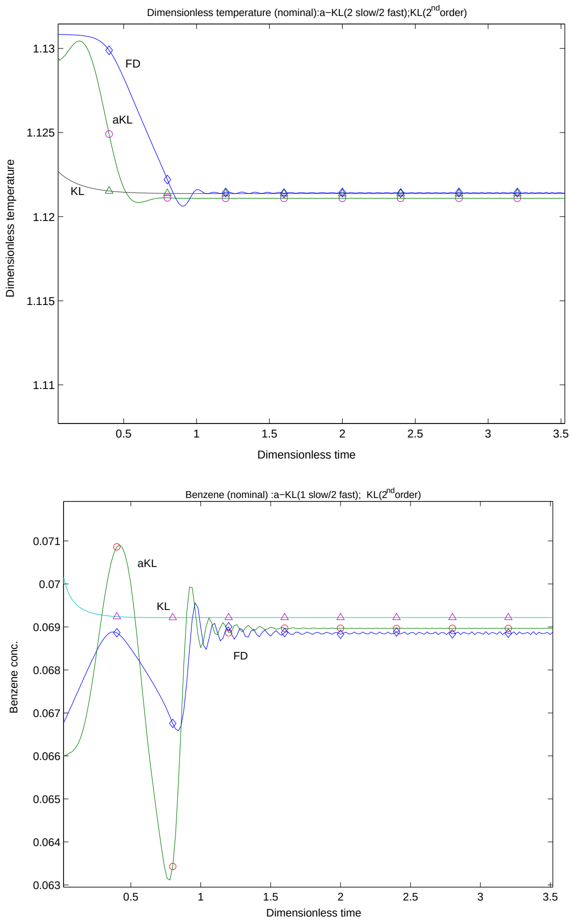

Fig. 2. Model fit at the nominal conditions.

4. SUMMARY

This work has introduced and demonstrated a nonlinear Galerkin method based on the work of (Sirovich *et al.*, 1990) who introduced the concept of empirical eigenfunctions (EEFs). However, whereas the usual concept of the EEFs in the Galerkin method results in a linear solution, the use of accelerated EEFs (aEEFs) captures some of the fast modes that are ignored in the development of the linear solution. For highly non-linear systems, it is argued that the fast modes contain some of the nonlinear behavior and therefore their use in the development of a reduced-order model may produce a better representation.

In some ways the formulation presented in this work is similar to the Approximate Inertial Manifold (AIM) solution. The AIM solution is obtained by sequential substitution, assuming a pseudo-steady state for the fast modes. In the present work, such an assumption does not hold. The aKL-Galerkin method was then demonstrated on a highly non-linear tubular reactor system. The fit of the temperature and benzene models were compared to the finite difference solution. It was found that the aKL-Galerkin solution tracked the finite difference solution better than the KL-Galerkin solution. This may be crucial in control

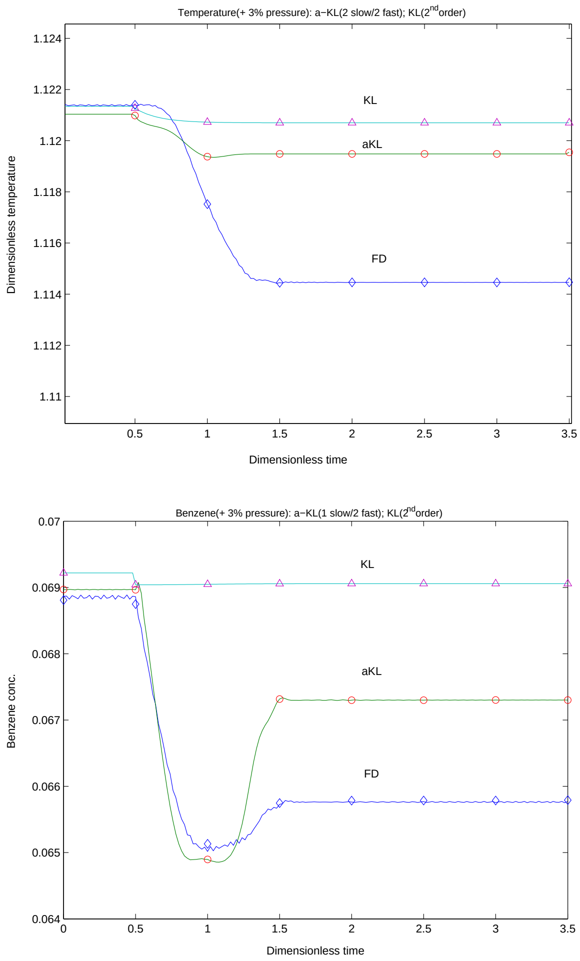

Fig. 3. Model fit: +3% in the reactor pressure.

applications where very tight control has to be maintained.

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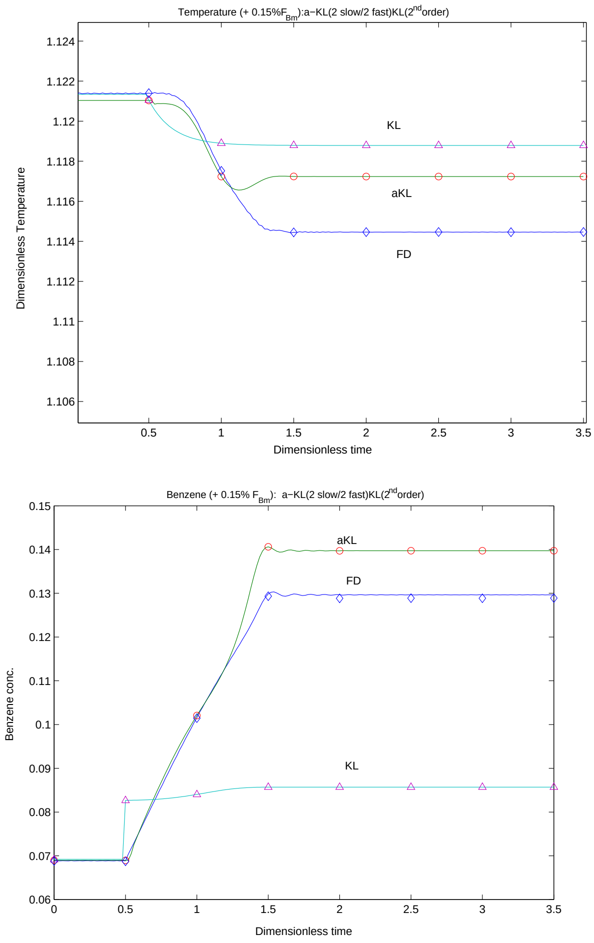

Fig. 4. Model fit: 0.15% in the benzene injection.

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