Application of POD to the nonlinear analysis of periodically forced chemical reactors

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1 Introduction

In the last 30 years, the real advantages of forced unsteady–state operations over conventional steady–state regimes of catalytic fixed–bed reactors have been widely supported. Special attention has been devoted to Reverse Flow Reactors (RFR) for catalytic combustion characterized by the periodic inversion of the flow direction (Matros & Bunimovich, 1996). The heat produced by the reaction is thus trapped in the central portion of the reactor; hence it is possible to conduct autothermal operation with gases containing low amounts of reactant.

Generally, the basic solution of periodically forced systems, such as RFR reactors, is a periodic solution with period equal to the forcing period, namely the double of the switch period. Furthermore, as model parameters are varied, a cooled RFR can exhibit very complex dynamic behaviour such as multiple stable solutions, subharmonic, quasi–periodic and chaotic solutions (e.g. Řeháček et al. 1998). Therefore, to properly design a RFR reactor, it is fundamental to foresee stability changes of regime solutions as model parameters are varied. This can be accomplished by means of bifurcation analysis via parameter continuation techniques. The RFR is, in general, described by a heterogeneous distributed model. In order to conduct the continuation analysis, the original infinite–dimensional PDE evolutionary equations are to be reduced to a finite–dimensional dynamical system, by means, for example, of orthogonal collocation on finite elements (Villadsen and Michelsen, 1978). Mancusi et al. (2003) conducted the numerical bifurcation analysis of the RFR by means of a properly constructed discrete map, based on the system's Poincaré map. This map is not available in analytical form and thus it, as well as its Jacobian, must be computed numerically; they also pointed out that most of the computation time is spent during repeated time integrations of the map. This leads to the need of expressing the original model as a set of ordinary differential equations of the lowest possible order.

The Proper Orthogonal Decomposition (POD) approach delivers an optimal set of empirical basis functions from an ensemble of observations obtained either experimentally or from numerical simulation, which characterize the spatio–temporal complexity of the system. Obtained orthogonal functions can be afterwards used in a Galerkin projection of the original system and as a result a low–dimensional model can be developed (Lumley, 1967). In this work, we apply POD/Galerkin to a model of RFR. We analyze the performance of the method by comparing solutions from the reduced model with a "reference" numerical solution.

2 Mathematical model and POD analysis

The reverse flow catalytic combustor (Figure 1) is modelled by a one–dimensional distributed model considering heat and mass transfer resistance between the gas and the solid phase, axial dispersion in the gas phase and axial heat conduction in the solid phase and cooling through the reactor wall. Constant value of effectiveness factor is assumed. The dimensionless mass and heat balances, considering first order reaction on the solid catalyst phase, and the relevant boundary conditions:

$$\begin{cases} \dfrac{\partial y_g}{\partial t} = \dfrac{1}{Pe_m^g}\dfrac{\partial^2 y_g}{\partial z^2} + \left[\dfrac{\partial y_g}{\partial z} - 2g(t)\dfrac{\partial y_g}{\partial z}\right] + J_m^g\left(y_s - y_g\right) \\[2mm] \dfrac{\partial \theta_g}{\partial t} = \dfrac{1}{Pe_h^g}\dfrac{\partial^2 \theta_g}{\partial z^2} + \left[\dfrac{\partial \theta_g}{\partial z} - 2g(t)\dfrac{\partial \theta_g}{\partial z}\right] + J_h^g\left(\theta_s - \theta_g\right) - \varphi\left(\theta_g - \theta_w\right) \\[2mm] \dfrac{\partial \theta_s}{\partial t} = \dfrac{1}{Pe_h^s}\dfrac{\partial^2 \theta_s}{\partial z^2} - J_h^s\left(\theta_s - \theta_g\right) + B\eta \mathrm{Da}\left(1 - y_s\right)\exp\dfrac{\theta_s}{1 + \theta_s/\gamma} \\[2mm] J_m^s\left(y_s - y_g\right) = \eta \mathrm{Da}\left(1 - y_s\right)\exp\dfrac{\theta_s}{1 + \theta_s/\gamma} \end{cases}$$

$$z = 0: \quad \left.\dfrac{\partial y_g}{\partial z}\right|_0 - g(t)Pe_m^g y_g(0,t) = 0 \; ; \quad \left.\dfrac{\partial \theta_g}{\partial z}\right|_0 - g(t)Pe_h^g\left(\theta_g(0,t) - \theta_{feed}\right) = 0 \; ; \quad \left.\dfrac{\partial \theta_s}{\partial z}\right|_0 = 0$$

$$z = 1: \quad \left.\dfrac{\partial y_g}{\partial z}\right|_1 - \left(1 - g(t)\right)Pe_m^g y_g(1,t) = 0 \; ; \quad \left.\dfrac{\partial \theta_g}{\partial z}\right|_1 - \left(1 - g(t)\right)Pe_h^g\left(\theta_g(1,t) - \theta_{feed}\right) = 0 \; ; \quad \left.\dfrac{\partial \theta_s}{\partial z}\right|_1 = 0$$

The forcing $g(t)$ is a discontinuous periodic square wave with minimum period of is $T = 2\tau$ where τ is the period of switching and is equal to 1 for flow going from left to right and equal to 0 for reverted flow. A general approach for study the dynamical behaviour of periodically forced system is based on the Poincaré map P (e.g. Kuznetsov, 1998).
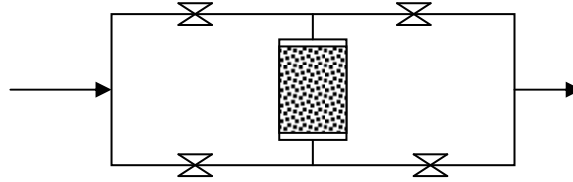

Figure 1. Schematic of a Reverse Flow Reactor

Parameter values for this work are: $\gamma = 16.68$, $Pe_m^g = 317.46$, $Pe_h^g = 644$, $Pe_h^s = 1.44\times10^5$, $\mathrm{Da} = 0.56$, $J_h^g = 28.4$, $J_h^s = 0.0227$, $J_m^g = 17.015$, $J_m^s = 22.9$, $\varphi = 0.72$, $\theta_w = -9.6$, $\eta = 1$, $B = 0.0097$, $\tau = 150$.

The PDE model is first approximated with finite differences and reduced to a system of ODE, which is then employed to build reference solutions by time integration. In the POD scheme, the objective is to determine a set of orthogonal basis functions which minimize, on average, the least square error between the truncated representation of the model and the "true" solution. By collecting time series obtained by simulation, the sampled data set is a vector–valued function given as a matrix:

$$U = \begin{bmatrix} u_1(x_1) & u_2(x_1) & \cdots & u_M(x_1) \\ u_1(x_2) & u_2(x_2) & \cdots & u_M(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ u_1(x_N) & u_2(x_N) & \cdots & u_M(x_N) \end{bmatrix}$$

where N is the number of positions in the spatial domain and M is the number of samples taken in time. A POD basis $\Phi = \{\varphi_1, \varphi_2, \ldots, \varphi_N\}$ is obtained by solving the eigenvalue problem $C\Phi = \lambda\Phi$ where $C(x, x') = \langle U_t(x), U_t(x')\rangle$ is the averaged autocorrelation matrix and angular brackets denote time–averaging operation. Using the POD modes, the solution $u_t(x)$ can be expressed as

$$\tilde{u}_t(x) = \sum_{k=1}^{K} a_k(t)\varphi_k(x)$$

where $K < N$ is the number of modes used for truncation, whereas $a_k(t)$ are modal coefficients that can be calculated by Galerkin projection of the original PDE on the POD modes. The ordering of the eigenvalues from

the largest to the smallest induces an ordering in the corresponding eigenfunctions, from the most to the least important.

3 Results and discussion

Figure 2 reports the solution diagram of this system obtained by parameter continuation, using the inlet temperature θ_{feed} as the bifurcation parameter. From left to right, periodic symmetric solutions occur until a pitchfork bifurcation (triangle) breaks the symmetry generating a pair of asymmetric periodic solutions. Then, on their branches, two secondary Hopf bifurcations (black squares) lead to a symmetric aperiodic regime (Russo et al, 2002). The three unstable branches (dotted lines) reconnect at a subcritical pitchfork bifurcation (triangle).
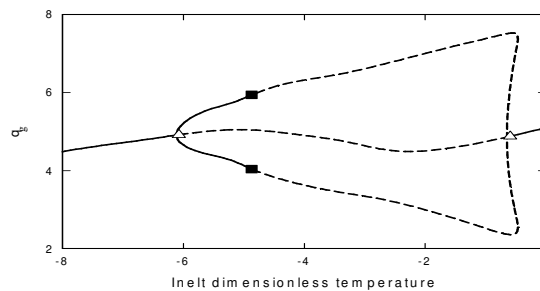

Figure 2 – Solution diagram. Bifurcation parameter: θ_{feed} .

The finite–difference solution with 50 nodes (150 ODE) obtained for $\theta_{feed} = -3$ (aperiodic solution) was used as reference ("true") solution and snapshots were collected and used to generate the POD basis functions. Then, simulations were conducted for $\theta_{feed} = -9$ (symmetric periodic solutions, Figure 3) and for $\theta_{feed} = -3$ (asymmetric quasi–periodic solutions, Figure 4).
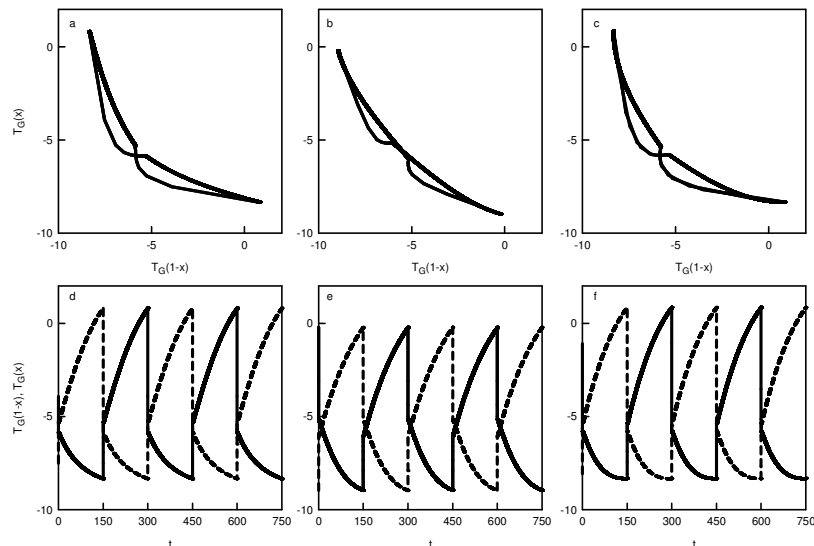

Figure 3 – Symmetric periodic regime at $\theta_{feed} = -9$. Orbit projections (top) and time series (bottom). Comparison among "true" solution (at left), POD with $N = 6$ (center) and POD with $N = 8$ (right).

It is seen that the periodic solution (Fig. 3) is well captured, both qualitatively and quantitatively, by just 8 basis functions, whereas qualitative agreement is achieved with as few as 6 basis functions. This even though the POD basis was constructed at a different value of the parameter ($\theta_{feed} = -3$ rather than –9). Only 30 ODE may thus be used in place of 150 for finite–difference ODE.

Quasi–periodic solutions, being more complex, as expected require a larger number of basis functions: Figure 3 shows that 15 basis functions are barely sufficient to reproduce the Poincaré map of the system as computed with 150 finite–difference ODE.
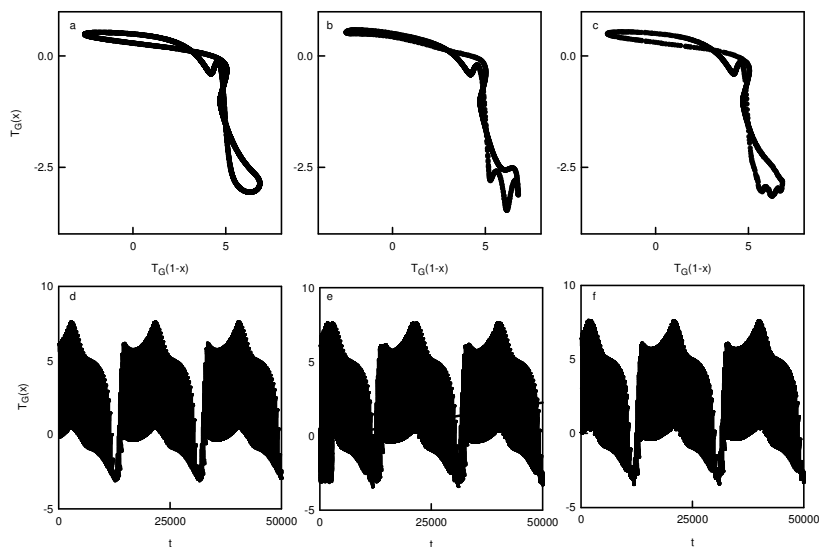

Figure 4 – Symmetric aperiodic regime at $\theta_{feed} = -3$. Poincaré maps (top) and time series (bottom). Comparison among "true" solution (at left), POD with $N = 8$ (center) and POD with $N = 15$ (right).

From these preliminary results, POD/Galerkin prove to be a promising approach to develop reduced models of periodically forced reactors like RFR. The advantage in order reduction can be beneficial in real–time applications such as model predictive control. Future work will be devoted to applications of POD reduced models in the bifurcation analysis of RFRs.

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