

# Empirical Reduction of Dynamical Reactor Models via Chaos Sampling: Comparison with Classic Reduction Methods.

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## 1 Introduction

Discretisation of science and engineering problems described by partial differential equations often yields discrete problems characterized by very high number of degrees of freedom, particularly in presence of nonlinearities in the governing equations – as most models of reactive systems contain. This may cause numerical solution to be very expensive – despite the continuously increasing computing power - both in terms of computational time and storage requirements. Hence, a strong need arises for model reduction techniques, yielding low-dimensional approximations of the full high- or infinite-dimensional systems while retaining their essential features.

The most popular approach in model reduction is a class of methods based on subspace projection. Methods based on this concept truncate the solution of the original system in the appropriate basis. Particularly, a quite common tool for model reduction and numerical analysis of the dynamics of chemical reactors are collocation methods, in which the systems' equations are approximated by polynomials with unknown coefficients, in chosen collocation points of the normalized domain [1]. Another classic approach for low order system determination is based on the Galerkin projection, which in its original form employs classic orthogonal functions as a basis. In some cases it can be much more efficient to use an empirically determined basis, containing a 'knowledge' about the systems' behavior. Such basis can be obtained by means of proper orthogonal decomposition (POD) [2], using a properly sampled ensemble of systems solutions obtained from more detailed numerical simulations. The main limitation of the POD method, when applied to the dynamic model reduction, comes from its strictly empirical character: usually POD employs sampled data from one transient evolution of the system to an asymptotic regime, whereas the process can often have more than one final state or regime as well as drastic changes of the solution upon changes in the system parameters. Hence, the first step of the procedure i.e., the collection of the representative set of simulation data, is considered to be crucial for generating a global basis. One possibility could be the determination of the POD basis from a single, but chaotic orbit, since such an orbit covers a portion of the phase space of higher dimension, it is expected to be characterized by a higher value of the information entropy, hence more information content about the system dynamics, if compared to lower dimensional periodic orbits.

In an earlier work [3] the chaos sampling approach with POD/Galerkin is demonstrated with the application to a typical system – a simple one-dimensional transient model of tubular reactor with

external heat recycle for energy recovery, which generates complex oscillatory solution profiles. In the present work, optimal construction of the POD basis is sought by sampling of the chaos window characterized by the maximum orbit entropy, in order to build a reduced order model able to capture the global attractor of the system. The performance of POD-based Reduced Order Models (ROM) are compared with those obtained with ROMs built using two classical approaches, i.e. approximation of the tubular reactor by means of the continuously stirred tank reactor (CSTR) cascade, and collocation on finite elements.

## 2 Mathematical model

The present study applies to the model of a pseudohomogeneous autothermal reactor with axial dispersion of mass and heat and external cooling. The model is essentially the one proposed in Ref. [4], where a comprehensive analysis of the dynamics of the system is presented, demonstrating the occurrence of complex oscillatory regimes – including periodic, multiperiodic and chaotic oscillations. Specifically, the authors studied the influence on the reactor dynamics of parameters such as the cooling medium temperature, the Lewis number, i.e. the measure of the pseudohomogeneity of the process, and the Peclet number characterizing mass and heat dispersion. The analysis of the effect of the Damköhler number on the dynamics of the adiabatic variant of the model can be found in Ref. [5].

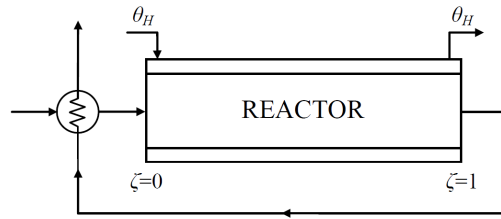


Figure 1. Schematic of the autothermal pseudohomogeneous reactor.

The dimensionless mass and energy balances of the system are:

$$\begin{aligned} \frac{\partial \alpha}{\partial \tau} + \frac{\partial \alpha}{\partial \zeta} &= \frac{1}{\text{Pe}_M} \frac{\partial^2 \alpha}{\partial \zeta^2} + \text{Da}(1-\alpha)^n \exp\left(\gamma \frac{\beta \theta}{1+\beta \theta}\right) \\ \text{Le} \frac{\partial \theta}{\partial \tau} + \frac{\partial \theta}{\partial \zeta} &= \frac{1}{\text{Pe}_T} \frac{\partial^2 \theta}{\partial \zeta^2} + \text{Da}(1-\alpha)^n \exp\left(\gamma \frac{\beta \theta}{1+\beta \theta}\right) + \delta(\theta_H - \theta) \end{aligned}$$

where  $\alpha$  is conversion degree and  $\theta$  is dimensionless temperature. The corresponding initial and boundary conditions are given, respectively, by:

$$\begin{aligned} \alpha(\zeta, 0) &= \alpha_0(\zeta); \quad \theta(\zeta, 0) = \theta_0(\zeta) \\ \alpha(0, \tau) &= \frac{1}{\text{Pe}_M} \frac{\partial \alpha}{\partial \zeta} \Big|_{\zeta=0}; \quad \theta(0, \tau) = \frac{1}{\text{Pe}_T} \frac{\partial \theta}{\partial \zeta} \Big|_{\zeta=0} + f \theta(1, \tau); \quad \frac{\partial \alpha}{\partial \zeta} \Big|_{\zeta=1} = 0; \quad \frac{\partial \theta}{\partial \zeta} \Big|_{\zeta=1} = 0 \end{aligned}$$

where  $f$  represents the efficiency of the effluent-feed heat exchange.

In the present work, the effect of the variation of temperature of the cooling medium  $\theta_H$  onto the system dynamics is considered. The other parameters are kept constant as follows:

$$\text{Da} = 0.15, \quad \beta = 1.4, \quad \delta = 2, \quad f = 0.3, \quad \text{Pe}_M = \text{Pe}_T = 300, \quad \text{Le} = 1, \quad n = 1$$

### 3 Reduction methods

Similarly as done in a previous work [6] where the mathematical model of a pseudohomogenous tubular reactor with mass recycle was analyzed by means of POD-based ROM, the PDE model is first reduced to a system of ODE by means of classical approximation using a cascade of  $N$  continuously stirred tank reactors (CSTRs) [7]. In practice, the reactor tube is divided into  $N$  pieces, which are treated as identical CSTRs, where thermal and concentration conditions in the  $(i)^{\text{th}}$  tank are taken as inlet conditions into the  $(i+1)^{\text{th}}$  tank. The number of tanks in the CSTR cascade was set to  $1/2 \text{ Pe}$ , where  $\text{Pe}$  is the Peclet number.

For further model reduction, a POD/Galerkin method with chaotic sampling, and orthogonal collocation on finite elements [1], were used. The POD technique delivers a optimal, in  $L^2$  sense, set of empirical orthogonal functions basing on the spatiotemporal set of data obtained from the experiment or the full order model numerical solution [2],  $u(x,t)$ , where  $t$  denotes time and  $x$  denotes position in space. The sampled data can be represented in the matrix form as:

$$U = \begin{bmatrix} u(x_1, t_1) & u(x_1, t_2) & \cdots & u(x_1, t_M) \\ u(x_2, t_1) & u(x_2, t_2) & \cdots & u(x_2, t_M) \\ \vdots & \vdots & \ddots & \vdots \\ u(x_N, t_1) & u(x_N, t_2) & \cdots & u(x_N, t_M) \end{bmatrix}$$

where  $N$  is the number of discretization points in spatial domain and  $M$  is the number of samples taken in time. The POD basis  $\Phi = \{\varphi_1, \varphi_2, \dots, \varphi_N\}$  is then determined by solving the eigenvalue problem  $C\Phi = \lambda\Phi$ , where  $C$  is the time-averaged autocorrelation matrix, i.e.  $C = U U^T$ , with an angular brackets denoting time-averaging operation. Using the determined POD functions, the truncated solution  $\tilde{u}(x,t)$  can be expressed as the linear combination of modes and time dependent coefficients as:

$$\tilde{u}(x,t) = \sum_{n=1}^K a_n(t) \varphi_n(x)$$

where  $K \ll N$  is the truncation order, i.e. the number of modes employed, whereas  $a_n(t)$  are modal coefficients to be determined by means of classical Galerkin method [8].

In the orthogonal collocation method on finite elements, the spatial domain is divided into  $m$  equally sized elements and within each element  $i$  we approximate the solution  $u_i$  by a weighted  $n^{\text{th}}$  order polynomial [1]:

$$\tilde{u}_i(x,t) = \sum_{j=1}^{n+1} l_{ij}(x) u_{ij}(t)$$

where  $l_{ij}(x)$  are Lagrange polynomials of order  $n$  defined on element  $i$ , and the weight  $u_{ij}$  is the state at the  $j^{\text{th}}$  discretization point within the element  $i$ . The collocation points  $x_{ij}$  are chosen as zeros of Legendre polynomials.

### 4 Results and discussion

In order to characterize the influence of the external cooling on the dynamics, brute force simulations were conducted in the range of  $\theta_H \in [-0.07, -0.02]$ , using CSTR-based model employing  $N=150$  tanks, hence resulting in a total of 300 ODE. Figure 2 presents a solution diagram, with bifurcation parameter  $\theta_H$ , obtained by plotting on the ordinates the extremes of the dimensionless temperature at the outlet of the reactor  $\theta_{ex}(1)$ . It can be seen that, for the  $\theta_H < -0.0605$ , the trajectories appears to have chaotic nature, and become periodic with increasing temperature of the cooling medium.

The idea is to generate samples for POD basis construction from the chaotic solution. In fact, the amount of ‘information’ included in the chaotic orbit is maximum; Figure 2 combines the solution diagram with the corresponding values – being a non-smooth function of the bifurcation parameter – of the orbit entropy, classically defined in the context of information theory as:

$$S = -\sum_{i=1}^N p_i \log_2 p_i$$

where  $p_i$  is the probability that the maximum value of the orbit falls into the  $i^{\text{th}}$  interval, and  $N$  is the number of intervals. If  $p_i=0$  then the value of the product  $p_i \log_2 p_i$  is assumed to be 0.

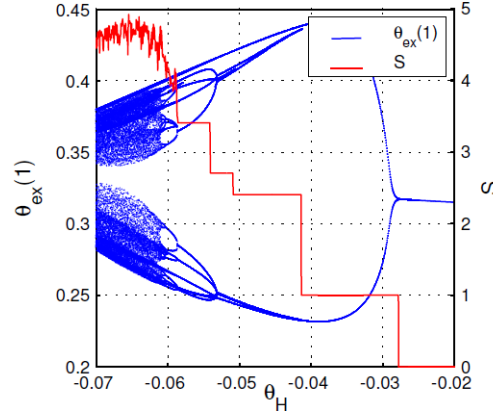


Figure 2. Effect of the cooling temperature  $\theta_H$  on the outlet temperature with the corresponding information entropy  $S$  of the orbit.

It can be seen (Fig. 2) that the entropy of the orbit increases gradually with increasing value of the orbits' periodicity, reaching highest values for values of  $\theta_H$  for which a chaotic character of the solution was observed. Moreover, it should be noted that, while values of entropy of periodic orbits are not influenced by the chosen value of  $N$ , the entropy of chaotic orbits tends to infinity with  $N \rightarrow \infty$ . Hence, with the purpose of determining a POD basis able to capture the global dynamics of the system, the solution trajectories were sampled at  $\theta_H = -0.065$ . Figure 3 shows a comparison of the chaotic attractors (for  $\theta_H = -0.065$ ) obtained by means of the 'full order model' (FOM, i.e. model base on CSTR cascade approximation, employing 300 ODE) and ROM built by the projection of the mass and energy balances onto 25 POD modes (resulting in total number of 50 ODE) – for each state variable - obtained from the chaotic orbit (POD-A/15). It can be seen that POD based model accurately approximate chaotic behaviour of the system.

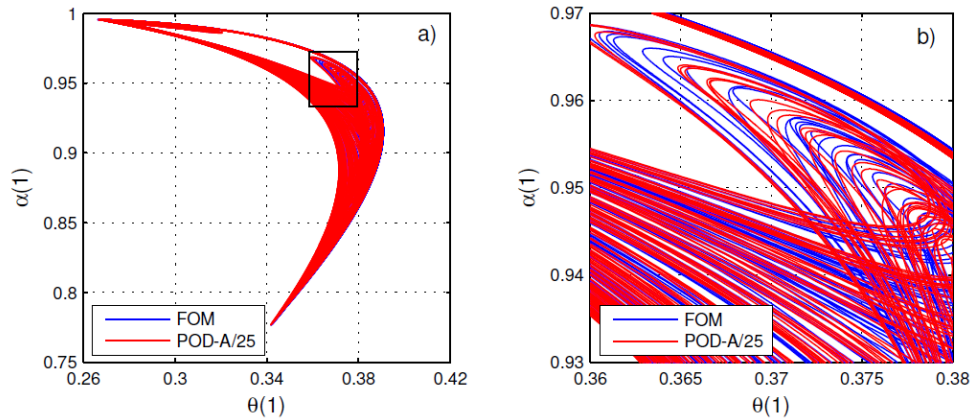


Figure 3. Comparison of chaotic attractors for  $\theta_H = -0.065$ : FOM vs POD-A/25 i.e., ROM obtained employing 25 POD basis functions determined from the chaotic orbit.

Further simulations employing ROMs reveals that the chaos-delivered basis (POD-A) performs very good even for lower values of  $\theta_H$ , where the solution trajectories are characterized by smaller complexity. As it can be observed in Figure 4, POD model approximates accurately the system behaviour both in the transient (Fig. 4a) and at steady state (Fig. 4b). On the other hand, when ROM based on the collocation method (employing 8 collocation points on each of the 3 finite elements) was used, significant divergence of the solution in the early transient was observed.

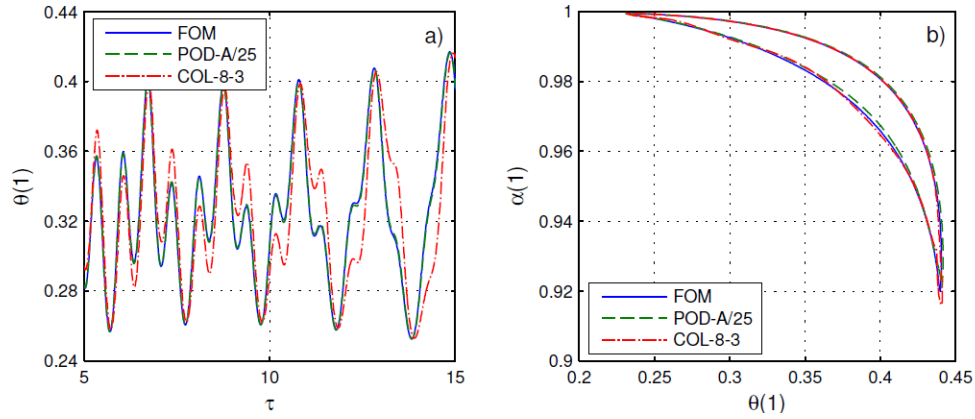


Figure 4. Comparison of the time series in early transient for  $\theta_H = -0.04$ : FOM vs POD-A/25 (POD basis determined at  $\theta_H = -0.065$ ) and orthogonal collocation on 3 elements with 8 nodes (a); corresponding limit cycles (b).

To verify quantitatively this rough visual finding, the distance between attractors was evaluated by means of the Hausdorff distance between sets defined as follows:

$$d_H(A, B) = \max\{dist(A, B), dist(B, A)\}$$

where  $dist(B, A) = \sup_{u \in B} dist(u, A)$  and  $dist(u, A) = \inf_{v \in A} \|u - v\|$

The error of the approximation evaluated in terms of the Hausdorff distance is marked on Figure 5: for the solution obtained at  $\theta_H = -0.04$  using chaotic basis (POD-A) and collocation based model (COL-8-3) and two additional POD-based ROMs: POD-B determined from multiperiodic oscillations at  $\theta_H = -0.055$  and POD-C determined at  $\theta_H = -0.04$  where period-one oscillations occurs.

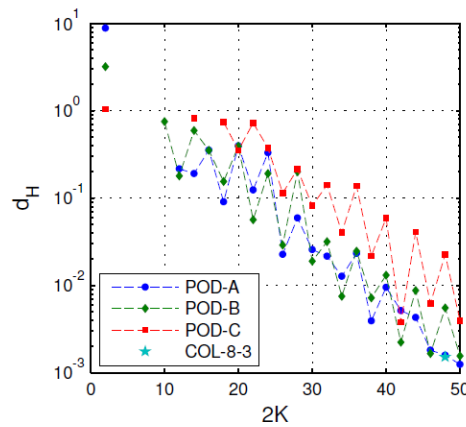


Figure 5. Hausdorff distance for  $\theta_H = -0.04$  between the attractor obtained by FOM and attractors obtained by means of three sets of POD bases, and orthogonal collocation on 3 elements with 8 nodes.  $2K$  denotes the total number of equations of the POD-based ROMs.

Table I reports the values of the Hausdorff distance computed for solutions obtained for two values of cooling temperature, namely  $\theta_H = -0.04$  and  $\theta_H = -0.065$  using all determined POD basis. In all cases, 25 modes were used for the approximation of each state variable in the ROM. As it is seen from Table 1, the error of the solution for  $\theta_H = -0.04$  obtained with POD-A/25 is more than 3 times smaller than the error obtained when the basis was constructed from the samples collected exactly at this value of the parameter. Obviously, for the chaotic trajectory the difference of the error produced by different POD models is much larger.

Table I: Hausdorff distance between the attractor of FOM solution and attractors obtained by means of four sets of POD bases. In bold the best solution.

POD basis	Entropy	$d_H$ $\theta_H = -0.04$ (periodic)	$d_H$ $\theta_H = -0.065$ (chaotic)
A/25 (chaotic)	4.78	<b>0.001250</b>	0.001811
B/25 (multiperiodic)	3.42	0.001556	0.004442
C/25 (periodic)	1	0.003935	0.011653
D/25 (fixed point)	0	0.147300	0.151094

## 5 Conclusions

A POD/Galerkin technique was successfully applied to the optimal reduction of the model of an autothermal tubular reactor with recycle. The empirical basis was constructed with data sampled in the highest entropy (chaotic) regime. As expected, the higher the entropy of the sampled orbits, the closer the approximation to the original model. POD/Galerkin is shown to perform better than the classic, efficient approach of orthogonal collocation on finite elements, especially in the early transient.

## References

- [1] Finlayson B. (1980). Nonlinear analysis in chemical engineering. McGraw Hill.
- [2] Holmes P, Lumley JL, Berkooz G. (1996). Turbulence, coherent structures, dynamical systems and symmetry. Cambridge University Press.
- [3] Bizon K, Continillo G. (2009). POD/Galerkin reduced order model of tubular reactor with heat recycle by sampling of chaotic orbits. 22<sup>nd</sup> ICDERS, Minsk, Belarus.
- [4] Berezowski M, Ptaszek P., Jacobsen EW. (2000). Dynamics of heat-integrated pseudohomogeneous tubular reactors with axial dispersion. Chem. Eng. Process. 39: 181.
- [5] Liu Y, Jacobsen W. (2004). On the use of reduced order models in bifurcation analysis of distributed parameter systems. Comp. Chem. Eng. 28: 161.
- [6] Bizon K, Continillo G, Russo L, Smuła J. (2008). On POD reduced models of tubular reactor with periodic regimes. Comp. Chem. Eng. 32: 1305.
- [7] Levenspiel O. (1998). Chemical reaction engineering. Wiley.
- [8] Hesthaven JS, Gottlieb S, Gottlieb D. (2007). Spectral methods for time-dependent problems. Cambridge University Press.