

# Identification of Low Order Tensorial Models for Tubular Reactors<sup>\*</sup>

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**Abstract:** In this paper we propose a novel procedure for obtaining a low order model of a large scale, non-linear process. The method is of generic nature. The efficiency of the proposed approach is illustrated on a benchmark example depicting industrial tubular reactor which are often used in petrochemical industries. The results show good performance of the proposed method. Our approach is based on the combinations of the methods of Proper Orthogonal Decomposition (*POD*), and non-linear System Identification techniques. It is showed here that the modal coefficient corresponding to the spectral decomposition of the system solutions can be viewed as the states of the reduced model. This has paved a way to propose a novel model reduction strategy for large scale systems. In the first step the spectral decomposition of system solutions is used to separate the spatial and temporal patterns (time varying modal coefficients) and in the second step a reduced model structure and it's parameters; linear and of non-linear tensorial (multi-variable polynomial) type are identified for approximating the temporal patterns obtained by the spectral decomposition. The state space matrices which happens to be the parameters of a black-box to be identified, appears linearly in the identification process. For the same reason, Ordinary Least Square method is used to identify the model parameters. The simplicity and reliability of proposed method gives computationally very efficient linear and non-linear low order models for large scale processes. The novel method also allows the way to compensate the mismatch between real plant and the reduced model outputs.

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## 1. INTRODUCTION

Industrial processes which are characterized by more than one independent variable, viz. space and time are often referred to as Distributed State Variable System (DSVS) or simply Distributed Systems (DS). Numerical solution techniques of such a system involve separation of spatial and temporal components. Spatial discretization of DS is done by means of Finite Volume or Finite Element methods (FVM or FEM) and Galerkin or Petro-Galerkin projection techniques. Although such discretizations approximate the dynamic process behavior reasonably well, it leads to very large order process model. It takes significant computational efforts (time, CPU requirement) to simulate such models and therefore such process models can not be used for online plant optimization and control purposes. Model Order Reduction (MOR) is therefore an important step before proceeding to control design, see e.g. Shvartsman and Kevrekidis [1998]. The method of Proper Orthogonal Decomposition (POD) or Principle Component Analysis (PCA) is widely used for deriving lower dimensional models from the First Principle rigorous Model (FPM). The POD method searches for dominant patterns in the given process and defines an optimal, data-dependent basis, that is subsequently used as a projection space to infer reduced order models through Galerkin type of projections, see Astrid [2004] and the references therein.

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POD methods are empirical (data dependent) in nature and therefore these methods are susceptible to changes in process inputs and process parameters. The reduced model obtained by POD techniques with Galerkin projections are usually very dense and one loses the original sparse model structure. Such a dense model structure and necessary evaluation of nonlinear function in original full dimensional space, does not always give computational advantage over original full scale FPM model, Nauta [2008], Astrid et al. [2008], Agudelo [2009]. This motivates one to look for other possible approaches which can give computationally efficient, reliable models which can be used for online control and optimization purpose. The other motivation for the method proposed in this paper lies in the fact that often it becomes impossible to get access to the discretized form of Partial Differential Equations (PDE) in commercial FPM software packages (simulators) and then one needs to explore other possible ways to infer reduced order models. One of such methods is explained in Wattamwar et al. [2010], which uses POD and system identification tools like N4SID algorithms, see e.g. Overschee and Moor [1996], Favoreel et al. [2000]. But the method proposed there results in local linear models which are not sufficient for approximating the non-linearities of large scale applications. Moreover in the method proposed there, the states of the linear reduced order model have no physical meaning. These reasons have motivated us to investigate another model reduction strategy, which is proposed here.

The method that is proposed here combines the theories from the field of system identification and model

reduction. Notions from the field of system identification like input/experiment design, parameter estimation, model structure selection etc. are used to infer reduced models from commercial simulators (FPM). In fact, the performance of the methods proposed here is comparable to the classical POD with Galerkin projection technique. The resulting reduced models do not need evaluation of nonlinear function in original full dimensional space, and therefore results into significant saving in computation time. Other advantages include, better structure of reduced model for the analytical treatment. In its earlier form the method presented here is applied on benchmark example of glass furnace which is a large scale application with significant complexity, Wattamwar et al. [2009]. The aim of the present paper is to refine the method and validate it on another large scale benchmark application which is tubular reactor in this case.

This paper is organized as follows. The overall methodology involving necessary tools from system theory like POD, a black-box type of system identification for linear and non-linear tensorial model is explained in section 2. The classical method of POD is explained first, which is subsequently correlated to the novel approach of identification based model reduction. The benchmark example of tubular reactor is explained in section 3. Some results of the proposed method on the motivation problem are presented in section 4 which is followed by future work and references.

## 2. THEORY BACKGROUND AND METHODOLOGY

One of the most promising and significant techniques for an efficient reduction of large-scale nonlinear systems characterized by existence of coherent patterns is the method of Proper Orthogonal Decompositions (POD) also known as the Karhunen-Loève method. Fluid dynamics is one of the first application of this technology, Holmes et al. [1996]. The method is based on the observation that evolution of dynamic process variables reveal coherent structures or *patterns* in many processes. This has led to the idea that the solutions of the model equations may be approximated by considering a small number of dominant coherent structures (called *modes* or *basis*) that are inferred in an *empirical* manner from measurements or simulated data. Given an ensemble of  $K$  measurements  $\mathbf{T}^k(\cdot)$ ,  $k = 1, \dots, K$  with each measurement defined on some spatial domain  $\Omega$ , the POD method amounts to assuming that each observation  $\mathbf{T}^k$  belongs to a Hilbert space  $\mathcal{H}$  of functions defined on  $\Omega$ . 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

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

Here, the  $a_j$ 's are referred to as the *modal coefficients* (MC) and the  $\varphi_j$ 's are the *modes* or *basis* of the expansion. The truncated expansion

$$\mathbf{T}_n(z) = \sum_{j=1}^n a_j \varphi_j(z), \quad z \in \Omega \quad (2)$$

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* in some norm over the complete ensemble is

$$\sum_{k=1}^K \|\mathbf{T}^k - \mathbf{T}_n^k\| \quad (3)$$

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  $R : \mathcal{H} \rightarrow \mathcal{H}$  that is defined as

$$\langle \psi_1, R\psi_2 \rangle := \frac{1}{K} \sum_{k=1}^K \langle \psi_1, \mathbf{T}^k \rangle \cdot \langle \psi_2, \mathbf{T}^k \rangle \quad (4)$$

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  $R$ , see e.g. Astrid [2004].

The POD modal coefficients are then obtained by the projection of the ensemble on the span of dominant POD modal coefficients as given by:

$$a_j(t) = \langle \varphi_j(z), \mathbf{T}_n(t, z) \rangle \quad (5)$$

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

$$\frac{\partial T_n}{\partial t} = \mathcal{A}(T_n) + \mathcal{B}(u) + \mathcal{F}(T_n, u, d) \quad (6)$$

and let  $\mathcal{H}_n$  denote an  $n$  dimensional subspace of  $\mathcal{H}$  and let  $P_n : \mathcal{H} \rightarrow \mathcal{H}_n$  and  $I_n : \mathcal{H}_n \rightarrow \mathcal{H}$  denote the canonical projection and canonical injection maps or operators respectively. The injection map brings back the system from reduced space to the full scale form of PDEs. The reduced model is then given by

$$P_n \frac{\partial T_n}{\partial t} = P_n \mathcal{A}(T_n) + P_n \mathcal{B}(u) + P_n \mathcal{F}(T_n, u, d) \quad (7)$$

where  $T_n(\cdot, t) = \mathbf{T}_n(t)$  belongs to  $\mathcal{H}_n = P_n \mathcal{H}$  for all  $t$ ,  $\mathcal{A}$  is the spatial operator for convection and diffusion, and is of linear nature  $\mathcal{B}$  defines input matrix and  $\mathcal{F}$  is nonlinear source term. In the specific case of a POD basis, the finite dimensional subspace  $\mathcal{H}_n = \text{span}(\varphi_1, \dots, \varphi_n)$  where the  $\varphi_j$ 's denote POD basis functions. In that case, (7) becomes an *ordinary differential equation* in the coefficients  $a_j(t)$  in the expansion of  $T_n$  as

$$\frac{\partial \langle P_n, T_n \rangle}{\partial t} = \mathcal{A} \langle P_n, T_n \rangle + \mathcal{B} \langle P_n, u \rangle + P_n \mathcal{F}(T_n, u, d) \quad (8)$$

or equivalently,

$$\frac{da_n}{dt} = \mathcal{A} a_n + \mathcal{B} \langle P_n, u \rangle + P_n \mathcal{F}(P_n^{-1} a_n, u, d) \quad (9)$$

The POD modal coefficients (MC)  $a_j(t)$  can also be viewed as the dominant temporal patterns along which the system evolves. The optimization problem to obtain POD basis as mentioned above in eq. (4) equivalently can also be solved for the ensemble  $\mathbf{T}_n$  as a 'Singular Value Decomposition' *SVD* which then gives POD basis function (*spatial patterns*) in the form of left singular vectors and POD modal coefficients (*temporal patterns* or *temporal dynamics*) as singular values multiplied by the right singular vectors. Modal coefficients are the states of

reduced order model. From the property of SVD these patterns are arranged as per their importance, i.e. the first POD basis corresponds to the direction of maximum energy and so will be the subsequent order. Usually a tolerance criterion based on amount of energy captured in the reduced model is applied to decide the truncation level or the span of POD basis as defined above in  $\mathcal{H}_n$ . The criterion is usually called projection energy and is given as below:

$$P_{tol} = \frac{\sum_{k=1}^n \lambda_k}{\sum_{k=1}^{\infty} \lambda_k} \quad (10)$$

where  $\lambda_k$  is the ' $k^{th}$ ' eigenvalue of the correlation operator as defined in eq. (4).

The first two terms of eq. (9) on RHS are linear and the third non-linear term do not appear for the systems defined by linear PDEs. For the system governed by linear PDEs the differential equation eq. (9) can be transformed in equivalent discrete time form as:

$$a_n(k+1) = A_d a_n(k) + B_d u(k) \quad (11)$$

At this point one can observe that given the ensemble  $\mathbf{T}_n$  one can obtain the POD basis  $\varphi_j(z)$  and the corresponding MCs  $a_j(t)$ . From the knowledge of MCs and system inputs ' $u$ ' the system parameters ' $A_d$ ' and ' $B_d$ ' in (11) can be easily estimated by least square estimation techniques. That is, equivalent reduced model can be obtained from the knowledge of states and inputs without invoking the model equations. This approach is very promising especially for many practical situations when the discretized version of governing PDEs used in commercial simulator are not easily accessible.

If one now think of the possible approach to identify the model parameters when the governing equations are of nonlinear form, as in eq. (9), one needs then some approximation for non-linear terms in the reduced space. There are many possible ways to describe the non-linearities like black-box, neural net, fuzzy logic, grey box as in see Romijn et al. [2008] and many other input-output based fit of Weiner-Hammerstein type. It is well known as well that the Taylor series expansion of a nonlinear function can be a good approximation of the non-linear function. If the aim is to approximate the linear system behavior then consideration of terms corresponding to the first derivative from the Taylor series alone is sufficient. But if the linear system is not sufficient enough then one must consider the higher terms in Taylor series that correspond to second derivatives and so on. Therefore the approximation of a non-linear function by linear and higher order terms from Taylor series will give a polynomial model form. But replacing the non-linear part by an equivalent polynomial expression for a multi-variable system is cumbersome due to the involvement of the tensor algebra (*Hessian computation*). For this reason we will briefly explain what does a Taylor series expansion for a scalar valued function means and then we will explain it for a vector valued function, and its implementation for computation purpose. Another reason for proposing a reduced dimensional polynomial type of a model to approximate the non-linear part of a full order model is that the polynomial systems have structure better suited for analytical treatment in the view of stability, controller and observer design requirements e.g. see Ebenbauer et al.

[2005]. For a *scalar* valued function,

$$\dot{x} = f(x), \text{ where } f: \mathcal{R} \rightarrow \mathcal{R} \ \& \ f(x^*) = 0 \quad (12)$$

Taylor series expansion in  $x$  as a nominal variable and  $\tilde{x}$  as a deviation variable,  $\tilde{x} = x - x^*$

$$\dot{\tilde{x}} = f(x^*) + f'(x^*)\tilde{x} + (1/2!)f''(x^*)\tilde{x}^2 + \dots \quad (13)$$

where,  $f'(x) = \mathcal{J}(x) : \mathcal{R} \rightarrow \mathcal{R}$ , the jacobian operator  $f''(x) = H(x) : \mathcal{R} \rightarrow \mathcal{R}$ , the Hessian operator.

For a *vector* valued function  $f : \mathcal{R}^n \rightarrow \mathcal{R}^n$ , the first derivative is defined as a map:  $f' : \mathcal{R}^n \rightarrow \mathcal{L}(\mathcal{R}^n, \mathcal{R}^n)$ , and when the first derivative is evaluated at  $x^* \in \mathcal{R}^n$  then  $f'(x^*) \in \mathcal{L}(\mathcal{R}^n, \mathcal{R}^n)$ , i.e.  $f'(x^*)$  is a linear operator, and when it acts on the ' $n$ ' dimensional vector ' $x$ ' then its image is  $\in \mathcal{R}^n$ , i.e.  $f'(x^*)(x) \in \mathcal{R}^n$ . This lets us to understand first derivative as a map,  $f' : \mathcal{R}^n * \mathcal{R}^n \rightarrow \mathcal{R}^n$ . As  $f'(x^*)$  is constant term (fixed operator), we better write it as  $[f'(x^*)](x) \in \mathcal{R}^n$ . The Jacobian operator is represented as,  $[f'(x^*)] := \mathcal{J}(x^*)$ .

The operator defined in the last expression can be written in terms of partial derivatives as,

$$[f'(x^*)](x) = \begin{bmatrix} \sum_{k=1}^n \frac{\partial f_1(x^*)}{\partial x_k} x_k \\ \vdots \\ \sum_{k=1}^n \frac{\partial f_n(x^*)}{\partial x_k} x_k \end{bmatrix} \quad (14)$$

The same procedure is repeated for computing the second derivative of the function, i.e.  $f'' : \mathcal{R}^n * \mathcal{R}^n * \mathcal{R}^n \rightarrow \mathcal{R}^n$ , i.e.  $[f''(x^*)] := H(x^*)$ , the Hessian operator. The Hessian operator is a tensor with argument from two domains while its codomain remains the same that of the Jacobian operator. The linearity of Hessian operator allows us to compute it like the Jacobian operator as in (14), but now with one more argument as:

$$[f''(x^*)](x, x) = \begin{bmatrix} \sum_{k=1}^n \sum_{j=1}^n \frac{\partial^2 f_1(x^*)}{\partial x_k \partial x_j} x_k x_j \\ \vdots \\ \sum_{k=1}^n \sum_{j=1}^n \frac{\partial^2 f_n(x^*)}{\partial x_k \partial x_j} x_k x_j \end{bmatrix} \quad (15)$$

the above expression can be written as:

$$[f''(x^*)](x, x) = A_1(x \otimes x) \quad (16)$$

where,  $(x \otimes x)$  is the Kronecker product.

The complete simplification procedure mentioned above is aimed to express,  $f'' : \mathcal{R}^n \rightarrow \mathcal{L}(\mathcal{R}^n, \mathcal{L}(\mathcal{R}^n, \mathcal{R}^n))$  as,  $f'' : \mathcal{R}^n \rightarrow \mathcal{L}(\mathcal{R}^{n^2}, \mathcal{R}^n)$ . This is possible due to the notion of the linearity of tensor operator.

From the discussion above, a nonlinear equation of the form  $\dot{x} = f(x, u)$  can be expanded in Taylor series as in (13) which can be approximated by a polynomial of the form,

$$\begin{aligned} \dot{x} = & Ax(t) + Bu(t) + A_1(x(t) \otimes x(t)) \\ & + B_1(u(t) \otimes u(t)) + Q(x(t) \otimes u(t)) \end{aligned} \quad (17)$$

Where,  $A_1, B_1, Q$  are equivalent Hessian operators and  $x \in \mathcal{R}^n, u \in \mathcal{R}^l, A \in \mathcal{R}^{n \times n}, B \in \mathcal{R}^{n \times l}, A_1 \in \mathcal{R}^{n \times n^2}, B_1 \in \mathcal{R}^{l \times l^2}, Q \in \mathcal{R}^{n \times (n * l)}$  and  $x(t) \otimes x(t), x(t) \otimes u(t), u(t) \otimes u(t)$  are the Kronecker products.

These methodological developments are based on full order simulator as the plant model, therefore we are not considering the output equations here.

Equivalent discrete form of Eq. (17) can be written as:

$$x(k+1) = A_d x(k) + B_d u(k) + A_{1d}(x(k) \otimes x(k)) + B_{1d}(u(k) \otimes u(k)) + Q_d(x(k) \otimes u(k)) \quad (18)$$

As we are considering the discrete identification problem here, for the convenience in remaining part of the paper we have dropped the superscript ‘d’ form eq. (18) and from it’s corresponding terms.

Note that the model equation (18) is non-linear in states and inputs but it is linear in all the system parameters (equivalent Jacobian and Hessian terms). The model in equation (18) is in fact tensorial model which is implemented in multi-variable polynomial form. The Kronecker product distinguishes the tensorial model from usual polynomial model. This is a big advantage. Because if the states and inputs are known then by fixing the above polynomial model structure we can estimate the system parameters by Least Square parameter Estimation (LSE) techniques.

Coming back to the problem of the reduced model identification, the states in (17) can be seen as POD modal coefficients (MC) and then linear and non-linear part in (9) can be approximated by (17).

Another interesting feature of the proposed framework is the ability to approximate the time-dependent variations of physical parameters of the process. To do so, the uncertain parameter should be treated similar to the process input and the corresponding process snapshots due to the parameter excitation need to be included while computing the POD basis functions and MCs. As per the knowledge of the author, this approach of model reduction for very large scale process under process parameter uncertainty is not thoroughly studied in the past.

Once the MC and POD basis are obtained from the full scale FPM (simulator) as mentioned earlier, then by using the tensors decomposition as in eq.(15) for eq.(17), the problem of polynomial model parameter identification is a least square estimation( *LSE*) problem and if we define,

$$\xi_k := \text{col}(x(k), u(k), x(k) \otimes x(k), x(k) \otimes u(k), u(k) \otimes u(k)) \quad (19)$$

then from (18),  $x_{k+1} \simeq \Theta \xi_k$  Where,  $\Theta = [A B A_1 B_1 Q]$  and define the parameter estimation error at each time instance as

$$e_{k+1} = x_{k+1} - \Theta \xi_k \quad (20)$$

similarly the estimation error that is minimized by LSE method over the complete simulation horizon is

$$E := [x_1 \dots x_N] - \Theta[\xi_0 \dots \xi_{N-1}] \quad (21)$$

equivalently,  $E := X - \Theta \Xi$

where,  $N$  is the number of samples and ,

$X \in \mathcal{R}^{n \times (N-1)}$ ,  $\Xi \in \mathcal{R}^{n \times (N-1)}$  and  $\Theta \in \mathcal{R}^{n \times (n+l+n^2+l^2+n^*l)}$

The least square solution will be

$$\Theta = X \Xi^T (\Xi \Xi^T)^{-1} \quad (22)$$

The complete CFD spatio-temporal information can be reconstructed by projecting back the solution of reduced model (18) on the span of dominant POD basis  $\mathcal{H}_n$ . The reconstructed states of full order model will be given by,

$$\tilde{T}_n(k) = I_n a_n(k) = P_n^{-1} a_n(k), \text{ or equivalently} \quad (23)$$

$$\tilde{T}_n(k) = \sum_{j=1}^n \phi_j^{-1} a_j(k) \quad (24)$$

As this study is based on software simulations, the outputs can be chosen as per the user choice. For our research purpose, we have chosen them close to the real life situation. The constructed output equations can be approximated as:

$$\tilde{y}(k) = C \tilde{T}_n(k) \quad (25)$$

The error involved here will be the sum of projection error and the statistical fit in the identification step to the few selected POD modal coefficients corresponding to the maximum energy content as per eq. (10). As  $\tilde{T}_n(k)$  is computed, and if the plant output information is available as well then parameter  $C$  in (25) can be estimated by least square estimation techniques to compensate the (reduced) model mismatch and the real plant. One of the problem with the reduced order tensorial (multi-variable polynomial) models is its spurious instability, which sometimes arises due to the polynomial nature of the underlying model. We have not investigated this issue in this paper.

### 3. BENCHMARK EXAMPLE: TUBULAR REACTOR

Tubular reactors are often used in chemical and petrochemical industries, especially for exothermic reactions. The large ratio of surface area to volume of tubular reactors offer fast heat exchange with cooling jacket. Moreover they can be easily operated due to the absence of any moving parts. These features makes tubular reactors an integral part of many chemical processes.

A dynamical model of a tubular reactor is 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 coupled partial differential equations. The system of equations can be classified as a system of non self-adjoint, parabolic PDE’s. This is a 1D benchmark problem and it might not exactly represent the real life situation characterized by 3D flow patterns, multiple reactions and different parameter values. The benchmark tubular reactor model used here assumes first order reaction.

$$\frac{\partial T}{\partial t} = \frac{1}{P_{eh}} \frac{\partial^2 T}{\partial z^2} - \frac{1}{L_e} \frac{\partial T}{\partial z} + \nu C e^{\gamma(1-\frac{T}{T})} + \mu(T_{wall} - T) \quad (26a)$$

$$\frac{\partial C}{\partial t} = \frac{1}{P_{em}} \frac{\partial^2 C}{\partial z^2} - \frac{\partial C}{\partial z} - D_a C e^{\gamma(1-\frac{T}{T})} \quad (26b)$$

which are subject to the mixed boundary conditions

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

Many tubular reactor models that occur in the literature can be adequately represented by this dimensionless model that describes material and energy balances in the reactor. The model with its parameter values are taken from Hoo and Zheng [2002].  $T(z, t)$  and  $C(z, t)$  are dimensionless temperature and concentration state variables, respectively, which are functions of time  $t$  and position  $z$ . Here,  $t \in \mathbb{R}_+$  is the temporal independent variable

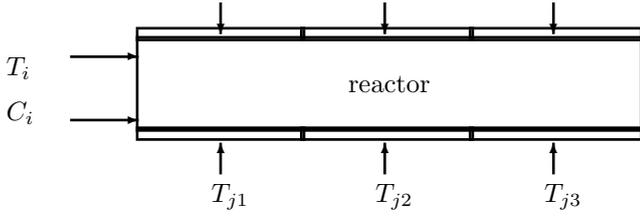


Fig. 1. Tubular reactor

and  $z \in \Omega := [0, 1]$  is the spatial independent variable. Inputs to the model are  $u(t) = \text{col}(T_{\text{wall}}(t), T_i, C_i)$  which are the wall temperature influenced by a heating/cooling jacket divided into three parts, the inflow temperature and the inflow concentration, respectively. Initial conditions at time instant  $t = 0$  are set to  $T_0(z) = T_{ss}$  and  $C_0(z) = C_{ss}$ , where  $T_{ss}, C_{ss}$  are steady states profiles. The physical parameters of the system are given in the table below.

Peclet number (energy)	Peh	5
Peclet number (mass)	Pem	5
Lewis number	Le	1.0
Damkohler number	Da	0.875
Activation energy	$\gamma$	15.0
Heat of reaction	$\nu$	0.8375
Heat transfer coefficient	$\mu$	13.0

#### 4. RESULTS AND DISCUSSION

The simulation results that are presented here are based on the CPU with configuration - Intel Core 2 CPU, T7200 @ 2.00 GHz, 2.00 GB of RAM, Microsoft Windows XP operating system.

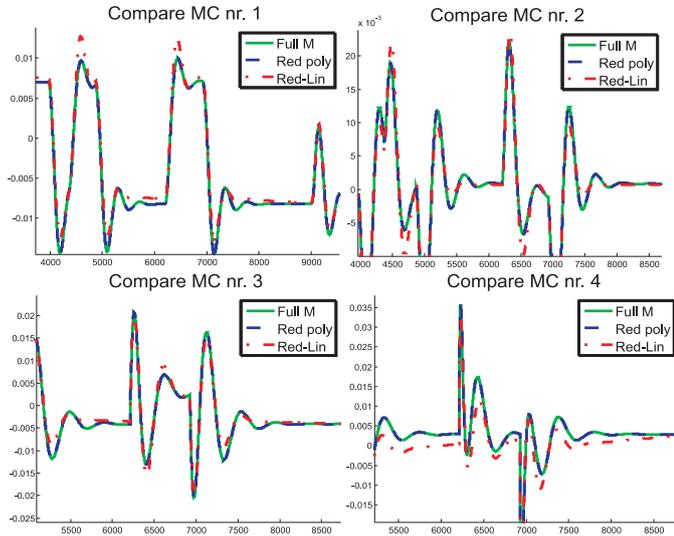


Fig. 2. Identification: Modal coefficients (MC), Tubular reactor, zoomed. ‘Red-Lin’ stands for ‘Reduced Order Linear model’, ‘Red-poly’ stands for ‘Reduced Order Polynomial model’, ‘Full M’ stands for ‘Full Order Non-linear model’, ‘nr.’ stands for ‘number’.

The spatial discretization of the 1-dimensional tubular reactor has been carried out with 100 grid cells. Since there are two states variables, temperature  $T$  and concentration  $C$ , the full scale model is of order  $n = 200$ . All variables in the equation (26) are represented in dimensionless form. The reaction kinetics is of first order. The full order model

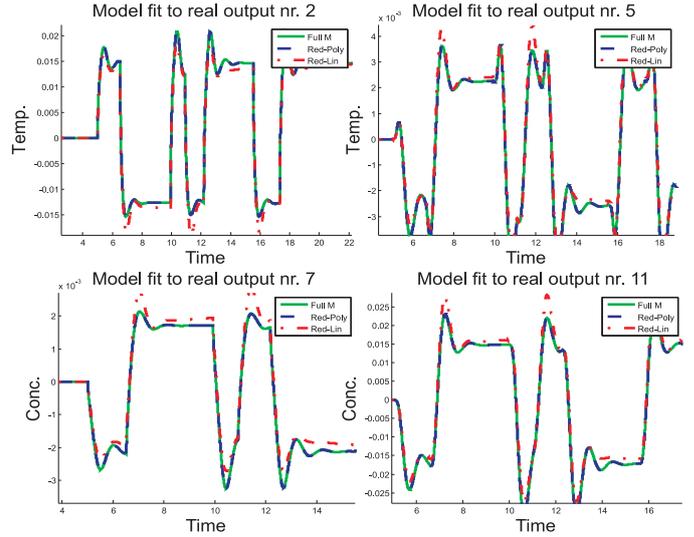


Fig. 3. Identification: Outputs, Tubular reac. zoomed

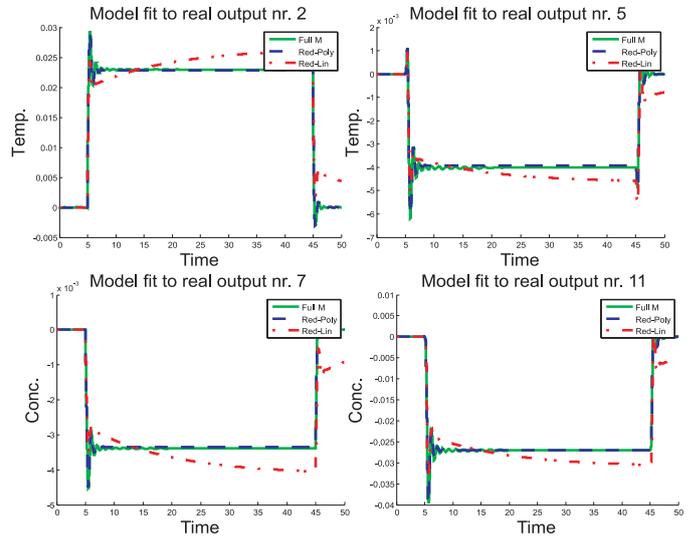


Fig. 4. Validation: Tubular reac.

has been simulated on a time horizon that corresponds to 50 times the residence time of the reactants in the reactor. The reaction was sampled for 20000 time samples. The time samples have been collected in a snapshot matrix and the POD basis functions have been computed. The results presented here are of the multi-variable case which means that the temperature and concentration state variables are stacked over each other in the snapshot matrix before computing the POD basis and modal coefficients. This ensures the coupling of the two state variables. We identified a linear model and a nonlinear second order tensor expansion model that maps inputs to modal coefficients.

Obviously, the quality of the identified model depends on the quality of the data. Therefore the data should be generated by input signals which excite the full scale model in the frequency range which is of the interest from a control point of view. The full model was excited with a Pseudo Random Binary Signal (PRBS) on  $T_i$ . PRBS fulfills the condition of persistence of excitation, which is necessary for getting a good identified model. The average switching time of such an identification signal should

usually be equivalent to the process time constant. But as all the variables are dimensionless, the time constant of the tubular reactor is small with respect to time constant of a real-life tubular reactor. Therefore, the average switching of PRBS signal was adjusted to 1/20 of the total simulation horizon. The initial condition was the steady state profile of temperature and concentration. As in real life situations, changes in input are implemented in the form of steps, the validation signal was a step input on  $T_i$ . The physical parameters of the full scale model are very close to an unstable operating condition. This is evidenced when a 3% amplitude change of inputs is taken from their nominal value. For the same reason, input signals for validation of the identified models are limited to 2% amplitude changes from their nominal value.

The fit of the reduced linear and the reduced tensor model to the first 4 modal coefficients, is shown in Figure 2. The full blue line represents the reduced linear model, the dash green line is reduced tensor model and the dash-dot green line is the full scale model. The reduced tensor model can fit 12 modal coefficients without becoming unstable. But this increases the computation time of the reduced model and therefore we fit the tensor expansion model to only 8 modal coefficients which captures > 99% of the projection energy. The plot shows that the linear reduced model does not fit as good as the reduced tensor model. The identification results for the real outputs are shown in Figure 3, while validation results are shown in Figure 4. The result presented here are based on software simulation alone and we assume that both, the temperature and the concentration can be measured at any location in the reactor. In all the figures the top plots show temperatures and the lower plots show concentrations in the reactor. Sensors 2<sup>nd</sup> and 7<sup>th</sup> are located at 10% of the reactor length from the left entrance while the sensors 5<sup>th</sup> and 11<sup>th</sup> are located at 20% from the reactor end i.e. right hand side end in Figure 1. Each identification plot shows the response of the three models viz. linear, tensor and full scale model. Although both the reduced order models show good performance, the reduced order tensor model fits the full scale model perfectly. The validation plot confirms the same conclusion. The reduced tensor model also captures the oscillations very well.

As explained in the last paragraph, depending on the number of modal coefficients fitted by the tensorial model, the computation time of the reduced order tensorial model can vary. For the tubular reactor, when 8 modal coefficients are fitted, the simulation time is approximately 30% that of the full order model.

## 5. CONCLUSION AND FUTURE RESEARCH

In this paper we have proposed a new model reduction method and its application on large scale industrial application. The proposed method is promising and suited especially for the very large scale processes where complexity reduction by using merely physical insight is not possible. Some other benefits of the proposed method include - method independent of model equations, better model structure, significant reduction in computation time etc.

We want to explore following topics in near future which has never/rarely been explored in literature like:

1. To investigate the possibility of imposing the stability in the identification process for the polynomial systems.
2. Exploitation of 'linear in parameter' model structure for the synthesis of controller and observers.
3. Implementation of the proposed method on industrial tubular reactors involving complicated physics and three spatial dimensions.
4. Studying the performance of the model in closed loop can be interesting as well.

## REFERENCES

- M. Agudelo. Positive polynomial constraints for pod-based model predictive controllers. *IEEE Transactions on Automatic Control, Special issue on Positive Polynomials in Control*, 54:988–999, 2009.
- P. Astrid. *Reduction of Process Simulation Models- A proper Orthogonal Decomposition Approach*. PhD thesis, Technical University of Eindhoven, 2004.
- P. Astrid, S. Weiland, K. Willcox, and A.C.P.M. Backx. Missing point estimation in models described by proper orthogonal decompositions. *IEEE Transactions on Automatic Control*, 53(10):2237–2251, 2008.
- C. Ebenbauer, R. Renz, and F. Allgower. Polynomial feedback and observer design using nonquadratic lyapunov function. *Conference on Decision and Control*, 2005.
- W. Favoreel, B. De Moor, and P. van Overschee. Subspace state space system identification for industrial processes. *Journal of Process Control*, 10:149–155, 2000.
- P. Holmes, J. L. Lumley, and G. Berkooz. *Turbulence, coherent structures, dynamical systems and symmetry*. Cambridge University Press: In Cambridge monograph on mechanics, 1996.
- K. A. Hoo and D. Zheng. Low-order model identification for implementable control solutions of distributed parameter systems. *Computers and Chemical Engineering*, 26(7:8):1049–1076, 2002.
- M. Nauta. *Model Reduction of a Lean NO<sub>x</sub> Trap Catalyst Model*. PhD thesis, Eindhoven University of Technology, Netherlands, 2008. ISBN 978-90-386-1376-5.
- P. Van Overschee and B. De Moor. *Identification for Linear Systems: Theory, Implementation, Applications*. Kluwer Academic, Dordrecht, The Netherlands, 1996.
- R. Romijn, L. Ozkan, S. Weiland, W. Marquardt, and J. Ludlage. A grey-box modeling approach for the reduction of nonlinear systems. *Journal of Process Control*, 18(9):906–914, 2008.
- S. Y. Shvartsman and I. G. Kevrekidis. Nonlinear model reduction for control of distributed parameter systems: A computer assisted study. *AIChE Journal*, 44(7):1579–1595, 1998.
- S. Wattamwar, S. Weiland, and T. Backx. Identification of low order models for large scale systems. *Proceedings of International Symposium on Advanced Control of Chemical Processes(ADCHEM)*, 2009.
- S. Wattamwar, S. Weiland, and T. Backx. Identification of low-order parameter-varying models for large-scale systems. *Journal of Process Control*, 20(2):158–172, 2010.