Complexity Reduction for Parametrized Catalytic Reaction Model

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***Abstract*—This work presents an application of a nonlinear model reduction approach to decrease the complexity in simulating a steady-state catalytic reactions, which are essential in facilitating many chemical processes. This approach is based on combining the proper orthogonal decomposition (POD) and the discrete empirical interpolation method (DEIM). This work illustrates the applicability of the POD-DEIM approach with the finite volume discretization. POD is used to generate a low dimensional basis set that captures the dominant behaviour of the solutions from the finite volume discretization with various parameter values, and hence provides a substantial reduction in the number of unknowns. Due to the nonlinearity of this problem, this work also applies DEIM to reduce the complexity in computing the POD projected nonlinear term. The numerical experiments demonstrate the accuracy and efficiency of these model reduction approaches through the parametric study of catalytic reactions.**

***Index Terms*—model reduction, differential equations, proper orthogonal decomposition, discrete empirical interpolation, catalytic reactions.**

I. Introduction

computer simulation recently has become an important tool to study many important phenomena in science and engineering that are inaccessible in the laboratory due to limitations in experimentation technology. This work considers steady-state behaviour of parametrized catalytic reactions, which play a crucial role in facilitating a wide range of chemical processes including steam reforming, ammonia synthesis, methanol synthesis, hydrocracking, and hydrodealkylation [1], [2].

To obtain accurate numerical solutions, the discretized dimension used in the simulation often requires to be very large, which can lead to an intense computational task. This work presents a computational reduction for the finite volume (FV) discretized system of catalytic reaction model by employing the projection-based technique that combines the methods of proper orthogonal decomposition and discrete empirical interpolation.

Proper orthogonal decomposition (POD) is a well-known approach to construct a basis that can maintain the physics of the original model with a much smaller dimension. POD is essentially the same as Karhunen-Love method and principal component analysis (PCA). It is often used together with the Galerkin projection process in model reduction context. Dominant dynamics of the systems can usually be captured in a very low-dimensional subspace of the POD basis. This approach has been used widely in many fields of science and engineering [3]. Although the resulting reduced system generally has much smaller number of unknowns compared to the original system, the complexity of the projected nonlinear term in this catalytic reaction model is still proportional to the dimension of the original one. The discrete empirical interpolation method (DEIM) [4] is therefore used to further approximate the nonlinear term in the form that can be computed efficiently. DEIM gives an efficient interpolatory projection approximation that allows only few important spatial locations to be evaluated. The combination of POD and DEIM approaches has been successfully used in many problems due to its applicability for general nonlinearlities, as demonstrated through various applications, such as in neuron modelling [5], shallow water equations [6], structural dynamics [7], electromagnetic wave scattering [8], subsurface flow [9], and many others [10], [11]. To the best of my knowledge, this POD-DEIM approach has not been used for the catalytic reaction problem. This work demonstrates the accuracy and efficiency of the POD-DEIM approach for the systems with varying 2-dimensional parameter values.

The remainder of this paper is organized as follows. The mathematical formulation of the catalytic reaction and the corresponding finite volume discretized system are given in Section II. The approach based on POD and DEIM for efficiently reducing the dimension of the FV discretized system is then discussed in Section III. Section IV presents the results generated from numerical simulation using the reduced systems with various parameter values. The conclusions of the study are finally summarized in Section V .

II. Problem Formulation

A catalytic reaction is a chemical reaction between reactants together with catalyst which will return to its original state after the reaction. The role of catalyst is to enable the reaction to happen. The primary reactant is usually a liquid or a gas. As the catalyst and the reactant are immiscible, the reaction occurs at the catalyst surface, which is therefore made as large as possible. This can be achieved by applying the catalyst to the pores of porous pellets. The reactant diffuses from the surface to the inside of the pellet. Meanwhile, being in contact with the catalyst, the reactant is converted to the final product. Assume that reactant A reacts in an equilibrium reaction with catalyst S at the pellet pore surface to the intermediate product AS in a way described by [1], [2], [12]

$$A + S \leftrightarrows AS$$

with concentrations of A, S, and AS, respectively, denoted by C_A mol/m^3, C_S mol/kg , C_{AS} mol/kg satisfying

$$C_{AS} = KC_AC_S \qquad \text{and} \qquad C_S = C_{S0} - C_{AS}$$

where K (m^3/mol) is a constant and C_{S0} is the initial concentration of the catalyst. It follows that

$$C_{AS} = \frac{KC_AC_{S0}}{1 + KC_A}.$$

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If AS reacts in a first order reaction to the final product B with reaction rate constant with reaction rate constant $\tilde{k}$, we have the reaction equation

$$\frac{\partial C_{AS}}{\partial t} = -\tilde{k}C_{AS} = -\tilde{k}C_{S0}\frac{KC_A}{1+KC_A} = k\frac{KC_A}{1+KC_A}.$$

This reaction acts as a source term for species B or, equivalently, as a sink term for A. To simplify the notation, let $C = C_A$ be the concentration of A inside a pellet. Under the additional assumption of a well-stirred fluid in order to maintain a constant concentration $C = C_R$ and $C_B = 0$ at the outer surface of spherical pellets where C_R is a fixed constant, R is the radius of each spherical pellet, and C_B is the concentration of the product B, the corresponding initial boundary value problem is given by

$$\frac{\partial C}{\partial t} - \nabla\cdot(D\nabla C) = -k\frac{KC}{1+KC}, \qquad 0<\tilde{r}<R, t>0, \quad (1)$$

$$C(r,0) = 0, \qquad 0<\tilde{r}<R, \quad (2)$$

$$C(R,t) = C_R, \frac{\partial}{\partial\tilde{r}}C(0,t) = 0, \qquad t>0, \quad (3)$$

where D is the diffusion coefficient of C inside the pellet. After a time $t \gg \max(R^2/D, (1+KC_R)/kK)$, the concentration C reaches stationary equilibrium. Supper that the pellet has spherical symmetry and the diffusion coefficient D is assumed to be constant. Then the catalyst reaction at equilibrium can be described by the following boundary value problem

$$D\tfrac{1}{\tilde{r}^2}\tfrac{d}{d\tilde{r}}\left(\tilde{r}^2\tfrac{dC}{d\tilde{r}}\right) = k\tfrac{KC}{1+KC}, \qquad 0<\tilde{r}<R, \quad (4)$$

$$C(R) = C_R, \quad \tfrac{d}{d\tilde{r}}C(0) = 0. \quad (5)$$

To make the problem dimensionless, we define

$$c := \frac{C}{C_R}, \quad r := \frac{\tilde{r}}{R}, \quad \lambda := \frac{kR^2}{DC_R}, \quad \alpha := \frac{1}{KC_R}$$

and the non-dimensionalized problem is given by

$$\tfrac{1}{r^2}\tfrac{d}{dr}\left(r^2\tfrac{dC}{dr}\right) = \lambda\tfrac{cH(c)}{\alpha+c}, \quad 0<r<1, \quad (6)$$

$$C(1) = 1, \quad \tfrac{dc}{dr}(0) = 0. \quad (7)$$

where H is the Heaviside function.

Next section discusses the numerical scheme that will be used to obtain the approximate solutions.

A. Finite Volume Discretized system

This section applies the finite volume method to construct the discretized system of the catalytic reaction problem. From (6), integrating over a control volume $V_j = (r_{j-\frac{1}{2}}, r_{j+\frac{1}{2}}) = ((j-\frac{1}{2})\triangle r, (j+\frac{1}{2})\triangle r)$, centred around the grid point $r_j = j\triangle r$ where $\triangle r$ is the grid size. Applying Gauss's theorem gives

$$\oint_{\partial V_j}\frac{\partial c}{\partial \mathbf{n}}dS = \int_{V_j} f(c)dV, \quad (8)$$

where

$$f(c) := \lambda\frac{cH(c)}{\alpha+c}, \quad (9)$$

and $\mathbf{n}$ is the outward unit normal on the boundary ∂V_j of the control volume. We next approximate both integrals above as follows

$$\oint_{\partial V_j} dS = \int_{r=r_{j+\frac{1}{2}}}\frac{\partial c}{\partial r}dS - \int_{r=r_{j-\frac{1}{2}}}\frac{\partial c}{\partial r}dS \quad (10)$$

$$= \frac{\partial c}{\partial r}(r_{j+\frac{1}{2}})4\pi r^2_{j+\frac{1}{2}} - \frac{\partial c}{\partial r}(r_{j-\frac{1}{2}})4\pi r^2_{j-\frac{1}{2}} \quad (11)$$

$$\approx \frac{4\pi}{\triangle r}\left(r^2_{j+\frac{1}{2}}(c_{j+1}-c_j) - r^2_{j-\frac{1}{2}}(c_j - c_{j-1})\right) \quad (12)$$

where c_j is the numerical approximation of $c(r_j)$, $r_j \in [0,1]$. Above integral approximations have used the midpoint rule with the central difference scheme to approximate the derivatives and used $\mathbf{n} = \mathbf{e}_r$ at radius $r = r_{j+\frac{1}{2}}$ of the sphere and $\mathbf{n} = -\mathbf{e}_r$ at radius $r = r_{j-\frac{1}{2}}$. Using again the midpoint rule approximates the volume integral in (8) gives

$$\int_{V_j} f(c)dV \approx f(c_j)|V_j| = \frac{4}{3}\pi f(c_j)\left(r^3_{j+\frac{1}{2}} - r^3_{j-\frac{1}{2}}\right). \quad (13)$$

From (12) and (13), the discretized system can be written in the form of

$$\frac{1}{\triangle r^2}\left(\beta_{j+\frac{1}{2}}(c_{j+1}-c_j) - \alpha_{j-\frac{1}{2}}(c_j - c_{j-1})\right) = f(c_j) \quad (14)$$

where $\beta_{j+\frac{1}{2}} := \frac{3r^2_{j+\frac{1}{2}}}{r^2_{j+\frac{1}{2}}+r_{j+\frac{1}{2}}r^2_{j-\frac{1}{2}}+r^2_{j-\frac{1}{2}}}$,
and $\alpha_{j-\frac{1}{2}} := \frac{3r^2_{j-\frac{1}{2}}}{r^2_{j+\frac{1}{2}}+r_{j+\frac{1}{2}}r^2_{j-\frac{1}{2}}+r^2_{j-\frac{1}{2}}}$.

Define a parameter vector $\mu = (\alpha, \lambda)$ and state variable vector of concentration $\mathbf{c}(\mu) = [c_1(\mu), \ldots, c_n(\mu)]^T \in \mathbb{R}^n$, where $c_j = c_j(\mu)$. The corresponding system of equations can be written in the matrix form as

$$\mathbf{A}(\mu)\mathbf{c}(\mu) + \mathbf{F}(\mathbf{c}(\mu);\mu) + \mathbf{b}(\mu) = 0, \quad (15)$$

where $\mathbf{A}(\mu) \in \mathbb{R}^{n\times n}$ and $\mathbf{b}(\mu) \in \mathbb{R}^n$ are constant matrix and vector, respectively, depending on parameter μ, and $\mathbf{F}(\mathbf{c}(\mu);\mu) = [F(c_1(\mu);\mu), \ldots, F(c_n(\mu);\mu)]$ is a componentwise nonlinear vector-valued function, where

$$F(c;\mu) = \lambda\frac{cH(c)}{\alpha+c} = \begin{cases} 0 & c<0 \\ \frac{\lambda c}{\alpha+c}, & c\geq 0 \end{cases}$$

as defined for f in (9) with additional dependence on parameter $\mu = (\alpha, \lambda)$. For a given μ, the equation (15) will be solved by Newton's method, which requires to use the Jacobian:

$$\mathbf{J}(\mathbf{c}(\mu);\mu) := \mathbf{A}(\mu) + \mathbf{J}_{\mathbf{F}}(\mathbf{c}(\mu);\mu), \quad (16)$$

where $\mathbf{J}_{\mathbf{F}}(\mathbf{c}(\mu),\mu)$ is a diagonal matrix given by

$$\mathbf{J}_{\mathbf{F}}(\mathbf{c}(\mu);\mu) = \mathrm{diag}\{F'(c_1(\mu);\mu), \ldots, F'(c_n(\mu);\mu)\} \in \mathbb{R}^{n\times n}$$

and the derivatives are taken with respect to the state variables $c_1, \ldots, c_n$.

$$F'(c;\mu) = \begin{cases} 0 & c<0 \\ \frac{\lambda\alpha}{(\alpha+c)^2}, & c\geq 0 \end{cases}.$$

Finally, the Newton's iteration update formula is of the form

$$\mathbf{c}^{i+1}(\mu) = \mathbf{c}^i(\mu) - [\mathbf{J}(\mathbf{c}^i(\mu);\mu)]^{-1}\mathbf{G}(\mathbf{c}^i;\mu),$$

where $\mathbf{G}(\mathbf{c};\mu) := \mathbf{A}(\mu)\mathbf{c}(\mu) + \mathbf{F}(\mathbf{c}(\mu);\mu) + \mathbf{b}(\mu)$.

To obtain accurate numerical solution, the dimension n of (15) is often required to be large, since it reflects the number

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of cell volumes used in the spatial discretization. Hence, solving these systems becomes computationally intensive, especially when many iterations are required to perform during Newton's method.

III. Complexity Reduction by Reduced-Order Modelling

A model reduction approach can be used to decrease this computational complexity. This work employs a projection-based model reduction approach. It first projects the dynamics of the system onto a low dimensional subspace to reduce the number of unknowns in the original problem. An effective and well-known approach called Proper Orthogonal Decomposition (POD), described in III-A is used to construct low dimensional subspace basis set, which will be used with the Galerkin projection. Since the complexity of projected nonlinear term is not truly reduced, as describe later in this section, the discrete empirical interpolation method (DEIM) will then be applied to fix this inefficiency as illustrated in Section III-B.

A. Proper Orthogonal Decomposition (POD)

Let $\mathbf{V}_k \in \mathbf{R}^{n\times k}$ be a k- dimensional basis matrix whose columns are orthonormal with $k \ll n$. Approximating the state variable $\mathbf{c}(t)$ in the span of $\mathbf{V}_k$, i.e. $\mathbf{c}(t) \approx \mathbf{V}_k\tilde{\mathbf{c}}(t)$, and enforcing the residual to be orthogonal to the space spanned by columns of $\mathbf{V}_k$ in the Galerkin projection give

$$\underbrace{\mathbf{V}_k^T\mathbf{A}(\mu)\mathbf{V}_k}_{\tilde{\mathbf{A}}(\mu)}\tilde{\mathbf{c}}(\mu) + \mathbf{V}_k^T\mathbf{F}(\mathbf{V}_k\tilde{\mathbf{c}}(\mu);\mu) + \underbrace{\mathbf{V}_k^T\mathbf{b}(\mu)}_{\tilde{\mathbf{b}}(\mu)} = 0, \quad (17)$$

with the corresponding Jacobian

$$\tilde{\mathbf{J}}(\tilde{\mathbf{c}}(\mu);\mu) := \tilde{\mathbf{A}}(\mu) + \mathbf{V}_k^T\mathbf{J}_{\mathbf{F}}(\mathbf{V}_k\tilde{\mathbf{c}}(\mu);\mu)\mathbf{V}_k, \quad (18)$$

where $\tilde{\mathbf{A}}(\mu) = \mathbf{V}_k^T\mathbf{A}\mathbf{V}_k \in \mathbb{R}^{k\times k}$ and $\tilde{\mathbf{b}}(\mu) = \mathbf{V}_k^T\mathbf{b}(\mu) \in \mathbb{R}^k$. The Newton's iteration formula is in the form:

$$\tilde{\mathbf{c}}^{i+1}(\mu) = \tilde{\mathbf{c}}^i(\mu) - [\tilde{\mathbf{J}}(\tilde{\mathbf{c}}^i(\mu);\mu)]^{-1}\tilde{\mathbf{G}}(\tilde{\mathbf{c}}^i;\mu),$$

where $\tilde{\mathbf{G}}(\tilde{\mathbf{c}};\mu) := \tilde{\mathbf{A}}(\mu)\tilde{\mathbf{c}}(\mu) + \mathbf{V}_k^T\mathbf{F}(\mathbf{V}_k\tilde{\mathbf{c}}(\mu);\mu) + \tilde{\mathbf{b}}(\mu)$.

POD is used to generate this basis matrix $\mathbf{V}_k$ by employing the solution *snapshots*, which are discrete samples of trajectories associated with a particular set of parameters. Let $\mathbf{C} := [\mathbf{c}_1, \ldots, \mathbf{c}_{n_s}] \in \mathbb{R}^{n\times n_s}$ be the matrix of snapshots $\mathbf{c}_j = \mathbf{c}(\mu_j)$, $\mu_j \in \mathcal{D}$ for $j = 1, \ldots, n_s$, with number of snapshots n_s and parameter domain $\mathcal{D} \subseteq \mathbb{R}^d$, $d > 0$. In a finite dimensional case, POD can be computed by using the singular value decomposition (SVD) of $\mathbf{C}$:

$$\mathbf{C} = \mathbf{V}\Sigma\mathbf{W}^T,$$

where $\mathbf{V} = [\mathbf{v}_1, \ldots, \mathbf{v}_r] \in \mathbb{R}^{n\times r}$ and $\mathbf{W} = [\mathbf{w}_1, \ldots, \mathbf{w}_r] \in \mathbb{R}^{n_s\times r}$ are orthogonal and $\Sigma = \mathrm{diag}(\sigma_1, \ldots, \sigma_r) \in \mathbb{R}^{r\times r}$ with $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_r > 0$. The POD basis of dimension k is then the set $\{\mathbf{v}_i\}_{i=1}^k$. More details on POD can be found in many previous works, e.g. [13], [3].

Notice that, when the Newton's iterations are performed, computing the term $\mathbf{V}_k^T\mathbf{J}_{\mathbf{F}}(\mathbf{V}_k\tilde{\mathbf{c}}(\mu);\mu)\mathbf{V}_k$, in the Jacobian of the reduced system (18) is required matrix-vector products to be done repeatedly with complexity depending on n, as the value of $\tilde{\mathbf{c}}(\mu)$ gets updated. Moreover, the low dimensional variable $\tilde{\mathbf{c}}(\mu)$ has to be prolonged back to the high dimensional vector in order to evaluate $\mathbf{F}(\cdot)$ and $\mathbf{J}_{\mathbf{F}}(\cdot)$. This computational inefficiency can be avoided by using the DEIM approximation described in the next section.

B. Discrete Empirical Interpolation Method (DEIM)

The DEIM approximation can be obtained by first computing a low-dimensional basis matrix $\mathbf{U} = [\mathbf{u}_1, \ldots, \mathbf{u}_m] \in \mathbb{R}^{n\times m}$ whose span gives a good approximation to the nonlinear snapshots $\{\mathbf{F}(\mathbf{c}(\mu_1)), \ldots, \mathbf{F}(\mathbf{c}(\mu_{n_s}))\}$, where $\mu_1, \ldots, \mu_{ns}$ are some selected parameter values and $m \ll n$. Then the interpolation indices $\wp_1, \wp_2, \ldots, \wp_n$ are obtained by a greedy procedure and used to approximate the nonlinear term $\mathbf{F}(\mathbf{V}_k\tilde{\mathbf{c}}(\mu))$ as follows:

$$\begin{aligned}\mathbf{F}(\mathbf{V}_k\tilde{\mathbf{c}}(\mu)) &\approx \mathbf{U}\mathbf{g}(\mu)\\ \mathbf{P}^T\mathbf{F}(\mathbf{V}_k\tilde{\mathbf{c}}(\mu)) &= \mathbf{P}^T\mathbf{U}\mathbf{g}(\mu)\\ \mathbf{g}(\mu) &:= (\mathbf{P}^T\mathbf{U})^{-1}\mathbf{F}(\mathbf{P}^T\mathbf{V}_k\tilde{\mathbf{c}}(\mu))\end{aligned}$$

where $\mathbf{P} = [\mathbf{e}_{\wp_1}, \ldots, \mathbf{e}_{\wp_m}] \in \mathbb{R}^{n\times m}$ and $\mathbf{e}_j$ is the j-th column of the identity matrix. Pre-multiplying $\mathbf{P}^T$ to a matrix is equivalent to selecting the rows $\wp_1, \wp_2, \ldots, \wp_n$ of that matrix. Hence, for a componentwise evaluation function $\mathbf{F}$, $\mathbf{P}^T\mathbf{F}(\mathbf{V}_k\tilde{\mathbf{c}}(\mu)) = \mathbf{F}(\mathbf{P}^T\mathbf{V}_k\tilde{\mathbf{c}}(\mu))$ as used above. That is, $\mathbf{V}_k^T\mathbf{F}(\mathbf{V}_k\tilde{\mathbf{c}}(\mu))$ can be approximated by

$$\widehat{\mathbf{F}}(\mathbf{V}_k\tilde{\mathbf{c}}(\mu)) := \underbrace{\mathbf{V}_k^T\mathbf{U}(\mathbf{P}^T\mathbf{U})^{-1}}_{\text{precomputed:}k\times m}\underbrace{\mathbf{F}(\mathbf{P}^T\mathbf{V}_k\tilde{\mathbf{c}}(\mu))}_{m\times 1}, \quad (19)$$

with the corresponding Jacobian given by

$$\widehat{\mathbf{J}}_{\mathbf{F}}(\tilde{\mathbf{c}}(\mu);\mu) := \underbrace{\mathbf{V}_k^T\mathbf{U}(\mathbf{P}^T\mathbf{U})^{-1}}_{\text{precomputed:}k\times m}\underbrace{\mathbf{J}_{\mathbf{F}}(\mathbf{P}^T\mathbf{V}_k\tilde{\mathbf{c}}(\mu))}_{m\times m}\underbrace{\mathbf{P}^T\mathbf{V}_k}_{m\times k}, \quad (20)$$

where the $m \times m$ Jacobian is given by

$$\mathbf{J}_{\mathbf{F}}(\mathbf{P}^T\mathbf{V}_k\tilde{\mathbf{c}}(\mu)) = \mathrm{diag}\{F'(\mathbf{c}_1^r(\mu)), \ldots, F'(\mathbf{c}_m^r(\mu))\},$$

and $\mathbf{c}^r(\mu) = \mathbf{P}^T\mathbf{V}_k\tilde{\mathbf{c}}(\mu)$, which can be computed with complexity independent of n as noted earlier. The Newton's iteration formula then becomes:

$$\tilde{\mathbf{c}}^{i+1}(\mu) = \tilde{\mathbf{c}}^i(\mu) - [\widehat{\mathbf{J}}(\tilde{\mathbf{c}}^i(\mu);\mu)]^{-1}\widehat{\mathbf{G}}(\tilde{\mathbf{c}}^i;\mu),$$

where $\widehat{\mathbf{G}}(\tilde{\mathbf{c}};\mu) := \tilde{\mathbf{A}}(\mu)\tilde{\mathbf{c}}(\mu) + \widehat{\mathbf{F}}(\mathbf{V}_k\tilde{\mathbf{c}}(\mu);\mu) + \tilde{\mathbf{b}}(\mu)$ and $\widehat{\mathbf{J}}(\tilde{\mathbf{c}}(\mu);\mu) = \tilde{\mathbf{A}}(\mu) + \widehat{\mathbf{J}}_{\mathbf{F}}(\tilde{\mathbf{c}}(\mu);\mu)$. As a result, the computational complexity for the approximation in (20) which is independent of n.

The algorithm for selecting the interpolation indices is analogous to the one proposed in [14] for constructing an approximation of a non-affine parametrized function with spatial variable defined in a continuous bounded domain.

To make this paper self-contained, the DEIM algorithm is given below. Note that the notation `max` in Algorithm 1 is the same as the function `max` in MATLAB. Thus, $[\rho\ \ \wp_\ell] = \max\{|\mathbf{r}|\}$ implies $\rho = |r_{\wp_\ell}| = \max_{i=1,\ldots,n}\{|r_i|\}$, with the smallest index in the case of a tie.

IV. Numerical Results

We consider the numerical solutions obtained from the original full-order system and the reduced systems described in the previous section. The spherical domain used in the dimensionless system is shown in 1.

The full-order system is solved by Newton method on the FV discretized system and 50 snapshots are sampled from the parameter domain $(\alpha, \lambda) \in [0.01, 10] \times [1, 100]$ (5 values of $\alpha \in [0.01, 10]$ and 10values of $\lambda \in [1, 100]$). The singular values of these solutions and nonlinear snapshots are

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Algorithm 1 : DEIM [4]

INPUT: $\{\mathbf{u}_\ell\}_{\ell=1}^m \subset \mathbb{R}^n$ linearly independent
OUTPUT: $\vec{\wp} = [\wp_1, \ldots, \wp_m]^T \in \mathbb{R}^m$

1: $[\rho \;\; \wp_1] = \max\{|\mathbf{u}_1|\}$
2: $\mathbf{U} = [\mathbf{u}_1]$, $\mathbf{P} = [\mathbf{e}_{\wp_1}]$, $\vec{\wp} = [\wp_1]$
3: **for** $\ell = 2$ to m **do**
4: Solve $(\mathbf{P}^T\mathbf{U})\mathbf{c} = \mathbf{P}^T\mathbf{u}_\ell$ for $\mathbf{c}$
5: $\mathbf{r} = \mathbf{u}_\ell - \mathbf{U}\mathbf{c}$
6: $[\rho \;\; \wp_\ell] = \max\{|\mathbf{r}|\}$
7: $\mathbf{U} \leftarrow [\mathbf{U} \;\; \mathbf{u}_\ell]$, $\mathbf{P} \leftarrow [\mathbf{P} \;\; \mathbf{e}_{\wp_\ell}]$, $\vec{\wp} \leftarrow \begin{bmatrix} \vec{\wp} \\ \wp_\ell \end{bmatrix}$
8: **end for**

shown in Figure 2. Figure 3 compares the numerical solutions of the concentration from the full-order system (dimension $n = 100$), POD reduced system (dimension $k = 10$)and POD-DEIM reduced system (dimension $k = 10, m = 10$) are indistinguishable. The concentration profiles from the reduced systems at different locations in the spherical domain are shown in Figure 4, together with the absolute error (compared to the solution from the full-order system) at different select parameter values that are not in the snapshots set, which are used to construct the reduced basis. Notice that when the dimension is reduced by a factor of 10, the absolute error is ranging between $\mathcal{O}(10^{-4})$ and $\mathcal{O}(10^{-2})$.

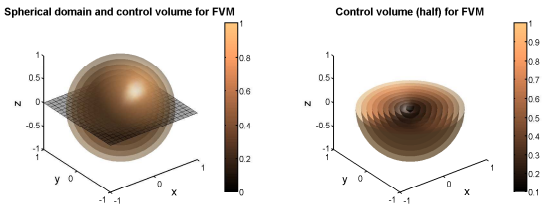

Fig. 1. Spherical domain (dimensionless) and the control volumes used in FV discretization.

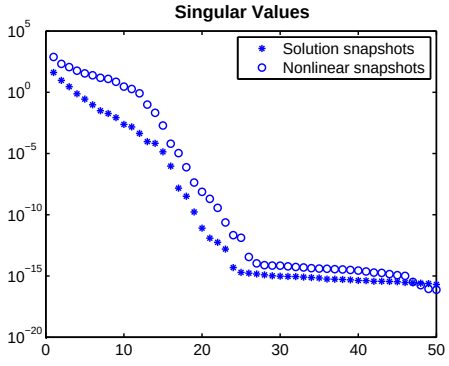

Fig. 2. Singular values of 50 solution snapshots and 50 nonlinear snapshots corresponding to different parameters $(\alpha, \lambda) \in [0.01, 10] \times [1, 100]$.

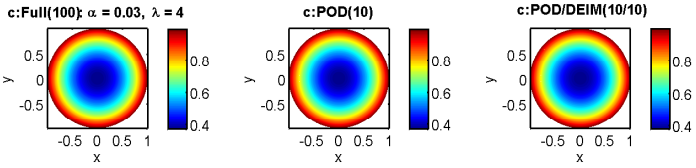

Fig. 3. Concentration computed from the original full-order system (dim=100) and from POD (dim=10) and POD-DEIM (dimPOD = dim DEIM =10) reduced systems using parameters $(\alpha, \lambda) = (0.03, 4)$, which are not in the snapshot set.

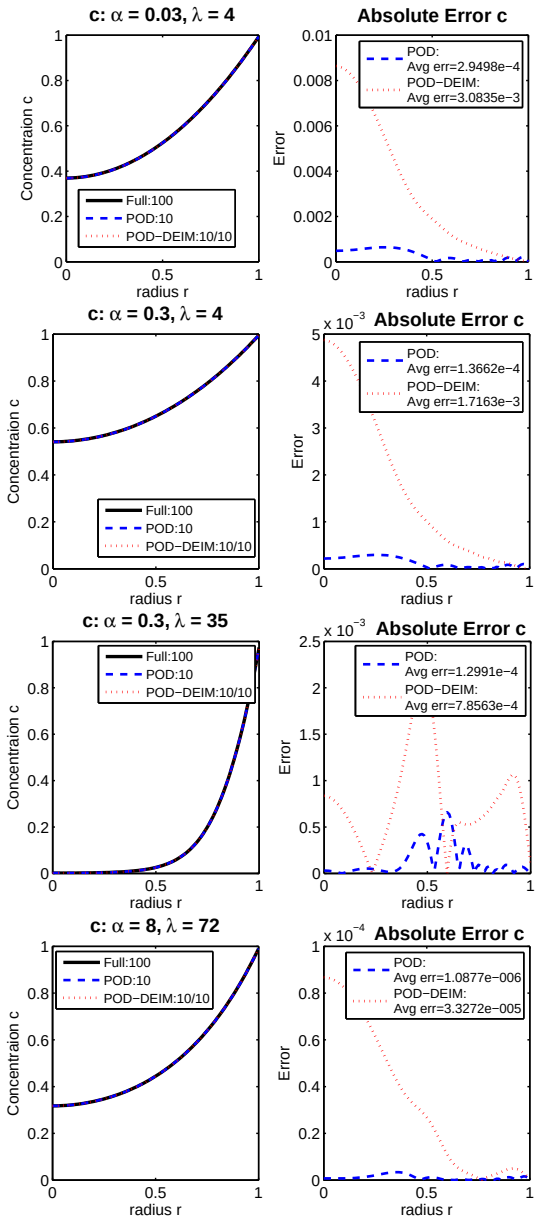

Fig. 4. Concentrations different values of parameters (α, λ), which are not in the snapshot set, computed from the original full-order system (dim=100) and from POD (dim=10) and POD-DEIM (dimPOD = dim DEIM =10) reduced systems with the corresponding absolute error.

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Table I shows the average relative errors of the POD-DEIM reduced systems using different 50 pairs of parameters (α, λ) where $\alpha \in \{0.0100, 2.5075, 5.0050, 7.5025, 10.0000\}$ and $\lambda \in \{1, 12, 23, 34, 45, 56, 67, 78, 89, 100\}$. Notice that the accuracy is improved as the dimensions of the reduce systems increase. The average relative errors of the solutions from POD-DEIM reduced systems are getting close to the ones obtained from the POD reduced system as the DEIM dimension increases. This illustrates the convergence of the POD-DEIM approach when it is applied to the systems arising from finite volume discretization.

TABLE I
Average relative errors of the solution of reduced systems of 50 pairs of parameters (α, λ) with $\alpha \in \{0.01, 2.5075, 5.005, 7.5025, 10\}$ and $\lambda \in \{1, 12, 23, 34, 45, 56, 67, 78, 89, 100\}$.

Dimension	Error (Average)
Full 100 (FV)	–
POD 10	3.9015×10^{-5}
POD 10/DEIM 10	2.1220×10^{-3}
POD 10/DEIM 20	3.9015×10^{-5}
POD 10/DEIM 30	3.9015×10^{-5}
POD 20	1.0617×10^{-13}
POD 20/DEIM 10	1.9698×10^{-3}
POD 20/DEIM 20	3.6521×10^{-13}
POD 20/DEIM 30	1.1768×10^{-13}
POD 30	1.0271×10^{-14}
POD 30/DEIM 10	1.9698×10^{-3}
POD 30/DEIM 20	3.4644×10^{-13}
POD 30/DEIM 30	1.4336×10^{-14}
POD 30/DEIM 40	1.0940×10^{-14}

V. Conclusion

This work illustrates the applicability of the model reduction approach based on POD and DEIM to decrease the complexity in solving the finite volume discretized system of catalytic reactions. The numerical results suggests that we can use this approach to accurately predict and analyze the concentration with much lower computational complexity, especially when the Newton's method is used. This approach can be extended to the inverse problem in which some certain parameters have to be identified.

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