A POD-DEIM Reduced Model for Compressible Gas Reservoir Flow Based on the Peng-Robinson Equation of State

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Abstract

The efficient simulation of gas flow in porous media is highly required in petroleum engineering, CO₂ sequestration, etc. However, it still remains a great challenge attributing to the gas compressibility compared with incompressible fluid flows. The commonly-used equation of states (EOS) of the gas are cubic equation and need to be updated in each iteration, and it also leads to the nonlinearity in flow equations, thus the computational cost mainly stems from the solution of gas EOS. In this paper, a hybrid reduced order model (ROM) coupling the proper orthogonal decomposition (POD) and the discrete empirical interpolation method (DEIM) is presented to accelerate the calculation of compressible single-phase gas reservoir flow, in which the Peng-Robinson EOS (P-R EOS) is considered to describe the gas states. To this end, in the hybrid ROM framework POD is applied to solve the flow equation and DEIM is used to solve the P-R EOS, respectively. The selection of POD modes and DEIM interpolation points, which plays a crucial role in the hybrid ROM, is discussed and carried out carefully. Performances of the proposed POD-DEIM-ROM are evaluated and demonstrated by two numerical cases. Simulation results illustrate that the proposed hybrid ROM displays a satisfactory computational speed-up (two orders of magnitudes faster) without sacrificing numerical accuracy significantly compared with the standard finite difference method. In addition, DEIM shows excellent acceleration and it is a perfect choice for solving the cubic gas EOS.

Keywords: Hybrid reduced order model , POD-DEIM , Compressible gas flow, Porous media , Peng-Robinson equation of state

1. Introduction

Natural gas is one of the most significant energy resources in the world. According to the World Natural Gas 2018-2050: World Energy Annual Report (Part 3) [1], the global natural gas production will continue rapidly increasing in the following 20 years, as shown in Figure 1. To improve the production efficiency and optimize the production period of natural gas, understanding the mechanism of the compressible gas flow in porous media is necessary. Thus, the compressible gas flow in porous media is one of the most fundamental problems in natural gas engineering, CO₂ sequestration in subsurface reservoirs, etc. Due to its crucial role, the efficient simulation of compressible gas flow in porous media is highly required in practical engineering and mechanism studies, which has gained increased attention in past several years and there exists a growing body of literature addressing this subject.

Figure 1: World historical and projected natural gas production (million tons of oil equivalent, 1980-2050) [1]

It is well known that the low cost, short period, and good repeatability compared with the experimental method are the main reasons why numerical simulations are irreplaceable tools in

production, optimization, and mechanism studies of natural gas resources [2]. Due to the compressibility of natural gas, the governing equations of fluid flow in porous media and equation of states of gas should be coupled and solved simultaneously in the simulation, which demonstrates a strong nonlinearity and takes most of the computational resources. Therefore, it still remains a great challenge to implement highly-efficient simulations of compressible gas flow in porous media. Many attempts have been made to study the acceleration techniques for solving the fluid flow in porous media efficiently, such as domain decomposition [3], parallel computing [4], multigrid method [5], etc., which have been widely used in past few years. It should be noted that in these methods, the degree of freedom (DOF, the number of values in the calculation that are free to vary) of unknowns remains unchangeable. Regardless of the introduced methods, much attention has recently been drawn towards applying the model order reduction method, it provides another alternative for fast calculation of nonlinear porous gas flow equations. The fundamental idea of this method is that instead of solving the original full-order problem with high DOF, a reduced order model in low dimensional space is established (always through Galerkin projection) and solved with low computational cost resulting in the substantial improvement of computational efficiency [6]. Generally, the commonly-used reduced order models can be classified into three types, one is local model order reduction, the main idea of this type methods is to construct coarse basis functions that approximate the solution on the coarse grid, such as up-scaling, multi-scale finite element method (MsFEM) [7], multi-scale finite volume method (MsFVM) [8], etc.; another is global model order reduction, in this type of methods the representative global snapshots are obtained and the best subspaces are constructed, it includes the proper orthogonal decomposition (POD) [9], dynamic mode decomposition (DMD) [10], discrete empirical interpolation method (DEIM) [11], etc.; and the last one is hybrid global-local model order reduction that combines the global and local model order reduction techniques, such as the work of Alotaibi et al. [12].

Many researches have been devoted to model order reduction approaches recently. Jenny et al. [13] presented a MsFVM to solve elliptic problems with different spatial scales for subsurface flow simulations, in which the effective transmissibilities were constructed locally to capture the local properties of differential operators. The applied approach was demonstrated to be conservative for fine-scale velocity fields and can treat tensor permeabilities and nonorthogonal grids correctly. Aarnes et al. [14] developed a hierarchical multiscale method (MsMFEM) based on the mixed finite element approach for simulations of two-phase incompressible flow in highly heterogeneous porous media with a wide span of length scales. The method was performed on nonuniform and unstructured coarse grids and the impact of large-scale features (such as traversing barriers and cross flow) was discussed. In addition, the local grid refinement/adaptation strategies were introduced to remedy the accuracy loss and improve the accuracy of the multiscale solution. Furthermore, Aarnes et al. [7] proposed a mixed MsFEM for solving stochastic flow equations with random coefficients in porous media. The main idea was to construct a low-dimensional approximation space for velocity by using the selected realizations of the permeability field. In their study, the normal Gaussian permeability field and exponential variogram permeability field were considered for validation. Vermeulen et al. [15] adopted the POD-ROM to a high-dimensional model inversion of transient nonlinear groundwater flow, results showed the POD-ROM was robust and efficient for a wide range of prior estimates and saved appreciable computational resources. Chaturantabut et al. [11] applied the POD and DEIM methods to simulate the non-linear miscible viscous fingering in a 2-D porous medium. In this method the POD was used to extract low-dimensional basis functions and construct the reduced-order model, and the DEIM was adopted to approximate the projected non-linear terms which were related with the original full-order dimension in the POD reduced order model. Gildin et al. [6] presented a POD-DEIM algorithm for reservoir simulations in which the large-scale partial differential systems were expected to be solved efficiently and robustly. An interpolation function called DEIM was used to handle the issues that nonlinear projections in POD were still dependent on the original full-order system. By using this technique, an original full-order model of 4050 state variables was reduced to the order 90 for POD-DEIM model, which showed the capability of solving complex subsurface flows by using a cheaper computational cost. Ghommam et al. [10] proposed to use global-local reduced modeling techniques for the simulation of flows in highly heterogeneous porous media. In their study, the numerical performances of the hybrid POD “GMsFEM model and DMD “GMsFEM model were

carefully evaluated from the perspectives of accuracy and robustness. Results illustrated the DMD “GMSFEM model shows much better prediction accuracy with significant model order reduction than that of POD “GMSFEM model, and the main reason can be attributed to the more powerful capability of DMD for extracting the dynamic information especially the relevant modes governing the long-time dynamics. Similarly, Alotaibi et al. [12] developed a global-local nonlinear model reduction method for solving high-contrast porous flows. To circumvent the expensive evaluation of projected nonlinear terms in resultant reduced-order models because of its dependence on the full dimension of the original system, the DEIM was employed to approximate the projected nonlinear functions on selected spatial points at offline step and online step. A substantial speed-up was benefited from the combination of both local and global mode reduction methods (GMSFEM and POD) along with using DEIM to cheaply compute the nonlinear terms. Kani et al. [16] developed a model order reduction technique based on deep residual recurrent neural network (DRRNN) for the forward uncertainty quantification of subsurface multiphase flows with random permeability distributions. The critical idea of this method was to use the POD and DEIM to reduce the computational complexity induced in high-fidelity simulations, and the DRRNN was applied to approximate the residual vector that was needed in the solution of nonlinear POD-DEIM formulation by using Newton iteration method. Therefore the complexity of the original nonlinear system was reduced by POD-DEIM and further reduced by DRRNN, which yielded a more attractive computational budget compared to conventional reduced order models. Based upon the above representative works, although the model order reduction methods have gained increased attention, it should be noted that above investigations all focused on the ROMs for incompressible flows in porous media. The development of model order reduction techniques in the presence of compressible flows is rarely reported.

Therefore, the model order reduction methods for compressible flows is still in its infancy and an exhaustive investigation of their potential for compressible flows is still lacking. The main challenge remains in the compressible flow is the nonlinearity induced by the compressibility. Lunati et al. [8] developed a modified multi-scale finite volume method (MsFVM) for compressible-flow problems to overcome the shortcoming of traditional MsFVM that is only effective for incompressible porous media and fluids. The principal idea of the modified MsFVM was to compute the local basis functions that were applied to extract the coarse-scale effective transmissibilities by using the same method for that of incompressible flows, and the effects of compressibility were considered in the solution of the coarse-scale pressure equation or in the reconstruction of fine-scale fluxes. Numerical examples demonstrated the accuracy of the proposed methods was affected by the modeling of compressibility. Krogstad et al. [17] presented a coarse grid localized model order reduction approach to speed up the simulation of compressible multiphase flow in porous media. In this approach the approximation of both flux and pressure fields was based on the POD coupled multiscale mixed FEM (MsMFEM) on the coarse grid. Numerical tests illustrated that the sparse basis POD is more process independent but it may result in more basis functions compared to standard POD models. Although the above works made a step towards the compressible porous flow, they all coupled the local model reduction and global model reduction techniques involving the calculation both on coarse grid and fine grid, and the multiple computation of different snapshots for local and global ROMs are also tedious, which complicate the solution process and program coding. To further explore the potential capability of reduced order modeling for fast simulation of compressible gas flow in porous media, in this paper a hybrid POD-DEIM global model is proposed considering the simplicity of the global model order reduction [18]. By applying this model, the computational burden associated with the solution of gas flow equation and equation of states of gas is expected to be mitigated substantially. The main contribution of this study is to couple the global model order reduction methods POD and DEIM in a hybrid ROM in the gas flow considering the Peng-Robinson EOS (P-R EOS), in which the POD is used to solve the flow equation and the DEIM is applied to solve the P-R EOS associated with the projected non-linear terms in the POD reduced system. Though the current work is still at initial stage and more efforts need to be paid, to the best of authors’ knowledge, there is rare report on the solution of EOS based on applying the DEIM.

The structure of this paper is organized as follows. In Section 2, the model problem is introduced in detail, including the equation of state of gas and the derivation of pressure equation. In Section 3, the conventional methodology for solving the model problem is shown. In Section 4, the establishment of

proposed POD-DEIM-ROM is presented, and the selection of POD modes and DEIM interpolation points is discussed. In Section 5, the proposed POD-DEIM-ROM is validated by two numerical cases and its reconstruction/prediction accuracy and computational speed-up are demonstrated. Concluding remarks of this work are summarized in Section 6.

2. Model problem

2.1. Governing equations

In this study, the compressible single-phase gas flow in porous media is considered as the model problem to introduce the proposed POD-DEIM-ROM. The governing equations of this model problem are described by the mass conservation equation, Darcy's law (by ignoring gravity's contribution) and equation of state, which are respectively given below,

$$\phi \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = q \text{ in } \Omega \quad (1)$$

$$\mathbf{u} = -\frac{\mathbf{k}}{\mu} \nabla p \text{ in } \Omega \quad (2)$$

$$pW = \rho ZRT \quad (3)$$

where ϕ is the porosity of the porous media; ρ is the gas density, kg / m^3 ; $\mathbf{u}$ is the Darcy velocity, m/s ; μ is the dynamic viscosity of gas, $\text{Pa}\cdot\text{s}$; $\mathbf{k}$ is the diagonal permeability, m^2 ; q is the mass accumulation rate in a control volume, $\text{kg} / (\text{m}^3 \cdot \text{s})$; p is the pressure, Pa ; W is the molecular weight of gas, kg/mol ; Z is the compressibility factor; R is the universal gas constant, $R = 8.314 \text{ J} / (\text{mol}\cdot\text{K})$; T is the temperature, K ; Ω represents the computational domain.

The following boundary conditions and initial conditions are adopted to close above governing equations,

$$\mathbf{u} \cdot \mathbf{n} = u_B \text{ on } \partial\Omega_N \quad (4)$$

$$p = p_B \text{ on } \partial\Omega_D \quad (5)$$

$$p = p_{\text{init}} \text{ or } Z = Z_{\text{init}} \text{ at } t = t_0 \quad (6)$$

where $\mathbf{n}$ represents the outward normal direction; the boundary velocity u_B , boundary pressure p_B and the initial pressure p_{init} and initial compressibility factor Z_{init} are all given parameters; The subscripts D and N denote the Dirichlet boundary and the Neumann boundary, respectively.

2.2. Peng-Robinson equation of state

To get the compressibility factor Z and solve Equation (3), the compressibility of the gas flow should be considered. Thus, the flow equation should be coupled with the equation of state (EOS) of gas. There are several choices for the EOS, such as Var der Waals EOS, Redlich-Kwong EOS, Soave-Redlich-Kwong EOS, Peng-Robinson EOS, and so on. In this work, the most popular equation of state describing natural gas flow in petroleum industry, Peng-Robinson EOS (P-R EOS), is applied to characterize the gas states in porous media. The typical form of P-R EOS reads,

$$p = \frac{RT}{v-b} - \frac{a(T)}{v^2 + 2bv - b^2} \quad (7)$$

For the convenience of computation, the P-R EOS can be reformulated as a cubic equation in terms of Z ,

$$Z^3 - (1-B)Z^2 + (A-2B-3B^2)Z - (AB-B^2-B^3) = 0 \quad (8)$$

In above equation, the parameters A and B are defined as follows,

$$A = \frac{a(T)p}{R^2T^2}, B = \frac{bp}{RT} \quad (9)$$

where $a(T) = a(T_c) \left(1 + m(1 - T_r^{0.5})\right)^2$, in which $a(T_c) = \frac{0.45724R^2T_c^2}{p_c}$, T_r is the reduced

temperature defined as $T_r = \frac{T}{T_c}$; $b = b(T_c) = \frac{0.0778RT_c}{p_c}$, T_c and p_c are critical temperature and

critical pressure, respectively; parameter m is computed by,

$$m = \begin{cases} 0.37464 + 1.54226\omega - 0.2699\omega^2, & 0 < \omega < 0.5 \\ 0.3796 + 1.485\omega - 0.1644\omega^2 + 0.01667\omega^3, & 0.1 < \omega < 2.0 \end{cases} \quad (10)$$

The acentric factor ω (a measure of the non-sphericity of molecules) of gas species in Equation (10) is defined as,

$$\omega = \frac{3}{7} \left(\log_{10} \left(\frac{p_c}{p_{\text{atm}}} \right) / \left(\frac{T_c}{T_b} - 1 \right) \right) - 1 \quad (11)$$

where p_{atm} is the atmosphere pressure; T_b is the boiling temperature.

2.3. Pressure equation

For the convenience of numerical solving, the original mass conservation equation (1) with primary unknown p is reformulated into a position-type equation regarding the pressure. To transform the mass conservation equation, the compressibility coefficient needs to be calculated first. The fluid compressibility coefficient at isothermal condition is expressed as,

$$c_f = \frac{1}{\rho} \left(\frac{\partial \rho}{\partial p} \right)_T \quad (12)$$

When P-R EOS is applied to describe the fluid state, the compressibility coefficient can be derived as,

$$c_f(Z) = \frac{1}{p} + \frac{1}{p} \frac{1}{Z} \frac{BZ^2 + (A-2B-6B^2)Z - (2AB-2B^2-3B^3)}{3Z^2 - 2(1-B)Z + (A-2B-3B^2)} \quad (13)$$

Substituting Equation (12) into the mass conservation equation (1) yields the following pressure equation,

$$\phi c_f(Z) p \frac{\partial p}{\partial t} = \nabla \cdot \left(p \frac{\mathbf{k}}{\mu} \nabla p \right) + \frac{ZRT}{W} q \text{ in } \Omega \quad (14)$$

3. Conventional methodology

Here the conventional numerical methods for solving the governing equations (14), (2), (8) and (13) of compressible single-phase gas flow in porous media are first briefly introduced. To solve this model problem, the semi-implicit and fully implicit algorithms can be applied. In this study, the semi-implicit algorithm is adopted due to its simple and easy implementation. Following semi-implicit algorithm, the governing equations (14) and (8) are solved implicitly and the equations (2) and (13) are solved explicitly. The numerical solving procedures are summarized as follows and the flow chart flow chart depicting the entire solution procedure is also presented in Figure 2,

Step 1: Give the initial calculation parameters, physical parameters and set the boundary conditions.

Step 2: Solve the P-R EOS (8) implicitly to get the compressibility factor Z . The Equation (8) is a cubic polynomial, the roots the Equation (8) can be found by using algebraic methods if the coefficients are real numbers.

Step 3: Calculate the compressibility coefficient c_f explicitly according to Equation (13).

Step 4: Solve the pressure equation (14) implicitly to get the pressure p with prescribed tolerance. In this work, the finite difference method (FDM) is applied to discrete the pressure equation (14), among which the second-order central difference scheme is used to discretize the second-order nonlinear term and the first-order difference scheme is adopted to discretize the unsteady term. The generated algebraic equations are solved by the Gauss-Seidel iteration and the numerical solution of pressure p can be obtained with prescribed tolerance.

Step 5: Calculate the Darcy velocity $\mathbf{u}$ explicitly according to Equation (2);

Step 6: Update the related variables, parameters and boundary values in the current time step;

Step 7: Go to the next time step and repeat steps 2 ~ 6 until the prescribed simulation time is reached.

Figure 2: The conventional semi-implicit algorithm based on FDM

From above numerical procedures shown in Fig. 2, it can be clearly seen that in step 2 and step 4 the P-R EOS (8) and pressure equation (14) need to be solved implicitly. Thus, the computational burden of this model problem mainly stems from the implicit solution of these two equations, namely, the iterative solution of pressure equation by using Gauss-Seidel method and the algebraic solution of P-R EOS by finding the roots of a cubic polynomial. Actually, the solution of P-R EOS takes most of the CPU time, this point will be demonstrated through the numerical examples in Section 5.

4. POD-DEIM reduced order model

To improve the computational efficiency of the conventional semi-implicit method shown in Section 3, a hybrid global reduced order model named POD-DEIM which combines the POD with DEIM is developed in this section. In the framework of POD-DEIM based semi-implicit algorithm, the POD is applied to solve the pressure equation (14) instead of the traditional iterative methods, and at the same time the DEIM is applied to solve the P-R EOS (8) instead of the conventional algebraic methods that used to determine the roots of cubic polynomial. Therefore, the degree of freedom of original model problem will be reduced substantially through the POD-DEIM-ROM. Owing to the low-dimension of POD-DEIM-ROM, the computational burden could be reduced significantly compared with directly solving the original model problem in a high-dimensional space. To clearly show the difference of the improved semi-implicit method based on POD-DEIM between the conventional semi-implicit method based on FDM, the entire solution procedure is briefly summarized in Figure 3.

Figure 3: The improved semi-implicit algorithm based on POD-DEIM

The cornerstone of the improved semi-implicit algorithm is to construct the POD-ROM-ROM. Therefore in the following content, the establishment of POD-ROM for pressure equation and the establishment of DEIM-ROM for P-R EOS are presented in detail, respectively.

4.1. POD-ROM for pressure equation

The pressure equation (14) can be discretized in the computational domain Ω using the standard finite difference method, finite volume method, etc. Suppose $n_x \times n_y$ uniform grids are used for the discretization in this work, the general form of the discrete pressure equation can be expressed as,

$$\mathbf{A}_{M \times M} \mathbf{p}_M = \mathbf{b}_M \quad (15)$$

where $\mathbf{A}_{M \times M}$ is the matrix of discrete coefficient with subscript $M = nx \times ny$ (noted that $\mathbf{A}_{M \times M}$ is a nonlinear matrix that depends on p and c_f); $\mathbf{b}_M$ is the matrix of discrete source term; $\mathbf{p}_M$ is the matrix of unknown pressure.

Suppose the pressure can be written as a combination of spectral coefficient $\mathbf{c}(t)$ and basis functions $\Phi(\mathbf{x})$: $\mathbf{p} = \mathbf{c}(t)\Phi(\mathbf{x})$, then Equation (15) is written as,

$$\mathbf{A}_{M \times M} \Phi_{M \times N} \mathbf{c}_N = \mathbf{b}_M \quad (16)$$

In order to establish the POD-ROM for pressure equation, the discrete pressure equation (16) will be projected into a low-dimensional space spanned by the selected N basis functions (or called POD modes) of pressure $\Phi_{M \times N}$ ($M \gg N$) using the projection. The basis functions of pressure can be obtained offline by the eigenvalue decomposition or singular value decomposition (SVD) of snapshots consisting of pressure samples at different evolution time. For those who are interested in more details of constructing the basis functions from snapshots, it is recommended to study the previous related kinds of literature [19]. Projecting Equation (16) into the low-dimensional space $\Phi_{M \times N}$ yields,

$$\Phi_{M \times N}^T \mathbf{A}_{M \times M} \Phi_{M \times N} \mathbf{c}_N = \Phi_{M \times N}^T \mathbf{b}_M \quad (17)$$

The above equation can be further rearranged as,

$$\tilde{\mathbf{A}}_{N \times N} \mathbf{c}_N = \tilde{\mathbf{b}}_N \quad (18)$$

where $\tilde{\mathbf{A}}_{N \times N} = \Phi_{M \times N}^T \mathbf{A}_{M \times M} \Phi_{M \times N}$ is the reduced order matrix of discrete coefficient with the subscript $N \ll M$; $\tilde{\mathbf{b}}_N = \Phi_{M \times N}^T \mathbf{b}_M$ is the reduced order matrix of discrete source term; $\mathbf{c}_N$ is the reduced order matrix of unknown spectral coefficient.

Equation (18) is the final POD-ROM for pressure equation (14), the spectral coefficients can be computed efficiently due to the low degree of freedom (DOF) of POD-ROM. In Table 1, the construction of POD-ROM for pressure equation is presented and summarized step by step. It should be noted that POD modes should be selected carefully because it can exert considerable effects on the prediction accuracy and speed-up of POD-ROM. In this study, the following accumulative energy contribution of different POD modes [20] is defined to determine the optimal POD modes number,

$$E_n = \sum_{j=1}^n \lambda_j \setminus \sum_{i=1}^N \lambda_i \times 100\% \quad (19)$$

where λ represents the eigenvalue obtained by the eigenvalue decomposition or SVD and is sorted in descending order; E_n is the accumulative energy contribution of the first n POD modes to the total energy of N POD modes.

Table 1: Construction of POD-ROM for pressure equation

Algorithm 1: POD-ROM		
Offline stage	1:	Solve the original pressure equation under different calculation conditions to obtain the representative snapshot ensembles of pressure
	2:	Compute the snapshot kernel and solve the eigenvalue problem using SVD or eigenvalue decomposition
	3:	Compute the basis functions
Online	4:	Project the discrete pressure equation into a low-dimensional space spanned by the

stage		selected basis functions and establish the POD-ROM
	5:	Compute the spectral coefficient by solving the POD-ROM
	6:	Reconstruct the pressure using the spectral coefficient and selected basis functions

4.2. DEIM-ROM for P-R EOS

From the original pressure equation (14), it is obvious to see that the first nonlinear term $\phi c_f(Z) p$ and the last nonlinear term $\frac{ZRTq}{W}$ are related to the compressibility factor Z . Thus, it will bring a problem that the POD-ROM (18) is still related to the original full-order model problem, which deteriorates the speed-up of POD-ROM. In order to settle this demerit of POD method with nonlinear terms, in this work the discrete empirical interpolation method (DEIM) [21] is applied innovatively, which is a newly developed model order reduction technique in 2010, to solve the P-R EOS in a reduced dimensional space that only depends on the selected interpolation points in the computational domain. The cornerstone of DEIM is to approximate the nonlinear function by projecting it onto a subspace that approximates the space generated by the nonlinear function and that is spanned by a basis of dimension $N \ll M$.

Suppose the first term and last term of pressure equation (14) can be expressed as a function of Z namely $f(Z)$, the approximation of $f(Z)$ can be formulated using DEIM as follows,

$$f(Z) \approx \tilde{f}(Z) = \mathbf{U}\mathbf{c} = \mathbf{U}(\mathbf{P}^T\mathbf{U})^{-1} \mathbf{P}^T \hat{f}(Z) \quad (20)$$

where $\hat{f}(Z)$ is calculated on selected interpolation points with DOF of N ; $\tilde{f}(Z)$ is the approximation of $f(Z)$ with DOF of M ($M \gg N$); $\mathbf{U}$ is the basis functions obtained by eigenvalue decomposition or singular value decomposition (SVD) of the snapshots of $f(Z)$; $\mathbf{P}$ is the interpolation point matrix.

It can be seen from Equation (20) that the P-R EOS can be solved only on selected interpolation points instead of in the whole computational domain, which greatly reduce the computational cost. A notable problem associated with DEIM-ROM of P-R EOS is that the computational efficiency and numerical accuracy strongly depend on the basis functions $\mathbf{U}$ and interpolation point matrix $\mathbf{P}$, which are both determined offline. When the basis functions $\mathbf{U}$ are determined, the selection of interpolation points is the key point and needs to be paid special attention. In this work, the DEIM algorithm originally proposed by Chaturantabut et. al [21] is used to select the representative interpolation points, as shown below in Table 2. From Table 2, actually it can be found that the interpolation points are selected where the interpolation error is the largest, interested readers can refer to [21] for more technical details.

Table 2: DEIM algorithm

Algorithm 2: DEIM-ROM
INPUT: $\{\mathbf{s}_l\}_{l=1}^m \subset \mathbb{R}^n$ linerly independent
OUTPUT: $\vec{\mathcal{J}} = [\mathcal{J}_1, \dots, \mathcal{J}_m]^T \in \mathbb{R}^m$
1: $[\theta , \mathcal{J}_1] = \max\{ \mathbf{s}_1 \}$
2: $\mathbf{U} = [\mathbf{s}_1], \mathbf{P} = [\mathbf{e}_{\mathcal{J}_1}], \vec{\mathcal{J}} = [\mathcal{J}_1]$
3: for $l = 2$ to m do

4:	Solve $(\mathbf{P}^T \mathbf{U}) \mathbf{c} = \mathbf{P}^T \mathbf{s}_l$ for $\mathbf{c}$
5:	$\mathbf{r} = \mathbf{s}_l - \mathbf{U} \mathbf{c}$
6:	$[\theta , \mathcal{J}_l] = \max\{ \mathbf{r} \}$
7:	$\mathbf{U} \leftarrow [\mathbf{U} \mathbf{s}_l], \mathbf{P} \leftarrow [\mathbf{P} \mathbf{e}_{\mathcal{J}_l}], \vec{\mathcal{J}} \leftarrow [\vec{\mathcal{J}} \mathcal{J}_l]$
8:	end for

5. Results and discussion

In this section, numerical simulations of two-dimensional single-phase natural gas flow (the main component of natural gas, methane, is considered) in porous media are performed to validate the computing performances of POD-DEIM-ROM through two cases. In numerical case 1, the reconstruction accuracy and acceleration effect of proposed POD-DEIM-ROM are displayed and evaluated; in case 2, the predictability of POD-DEIM-ROM is further verified and proofed. It should be mentioned that all simulations are carried out on an Intel Xeno E5-2640, CPU2.60 GHz PC with 64.00 GB of RAM in this work.

5.1. Numerical case 1

In case 1, the permeability distribution of porous media is shown in Figure 4, where the red color denotes a large permeability value k_1 and the blue color represents a small permeability value k_2 , respectively. For the setting of boundary conditions, the west boundary is set as high pressure p_1 and the east boundary is set as low pressure p_2 , the north and south boundaries are all set as Newman boundary with zero velocity. The initial pressure in the computational domain is set as p_0 . In this work, the sizes of the 2D computational domain are 100m×100m, and 100×100 uniform rectangular grids is used to discretize the domain. The prescribed simulation time is set as 30 days and the time step is set as 1.5×10^{-4} day. Detailed calculation parameters are presented in Table 3.

Figure 4: Permeability distribution in numerical case 1

Table 3: Calculation parameters in numerical case 1

Parameter	Value	Parameter	Value
ϕ	0.2	W	1.6×10^{-2} kg / mol
p_0	1.01325×10^5 Pa	μ	1.1067×10^{-5} Pa · s
p_1	1.01325×10^6 Pa	T	298 K
p_2	1.01325×10^5 Pa	$lx \times ly$	100 m × 100 m
k_1	1.0×10^{-1} D	$nx \times ny$	100 × 100
k_2	1.0×10^{-3} D	T_c	190.58 K
R	8.314 J / (mol.k)	T_b	111.63 K
q	0	p_c	4.604×10^6 Pa
Δt	1.5×10^{-4} day	simulation time	30 days

In order to obtain the pressure basis functions for constructing POD-ROM of pressure equation and the $f(Z)$ basis functions for selecting interpolation points in DEIM-ROM of P-R EOS, the representative pressure samples and $f(Z)$ samples need to be computed offline. In this work, these samples are supposed to be calculated using same parameter settings as shown in Table 3 in order to validate the reconstruction accuracy of POD-DEIM-ROM, where 1500 samples respectively for pressure and $f(Z)$ are considered.

5.1.1. Determination of POD modes and DEIM interpolation points

As mentioned in Section 3, the reconstruction and prediction accuracy as well as computational speed-up of POD-DEIM-ROM strongly depend on the selection of POD modes in POD-ROM and interpolation points in DEIM-ROM. Therefore, special attention should be paid on this issue. In order to accurately describe main characteristics of the model problem in this case, the truncation term of POD modes is supposed to be determined when 99.99% accumulative energy is captured. Figure 5 displays the variation of accumulative energy contribution with POD modes number. It can be clearly observed that 10 POD modes are enough to capture 99.99% accumulative energy, thus in this work 10 POD modes are adopted in POD-ROM. Based on the DEIM algorithm proposed by Chaturantabut et al. [21], 10 interpolation points are chosen in DEIM-ROM, as shown in Figure 6. It can be seen that most of the selected interpolation points gather around the zone where the permeability changes from large value to small value because the flow fields would change appreciably in this area. Results display that the relative error between the $f(Z)$ sample and the simulated $f(Z)$ by DEIM with 10 interpolation points is 2.39×10^{-3} , which can be ignored in the simulation. It should be noted that the trade-off between computational efficiency and numerical accuracy should be considered carefully when selecting the POD modes and interpolations points, this issue will be discussed at the end of this subsection in detail.

Figure 5: Variation of accumulative energy contribution with different POD modes

Figure 6: Selected interpolation points in DEIM-ROM, the indexes of these points are: (100, 50), (38, 53), (29, 71), (25, 50), (35, 67), (46, 50), (12, 50), (27, 27), (32, 31), (42, 58)

5.1.2. Results discussion

In this part, the simulation results of POD-DEIM-ROM are compared with those of standard finite difference method (FDM) which does not adopt any acceleration techniques. The reconstruction accuracy and computational speed-up of POD-DEIM-ROM are displayed and evaluated in detail. It is worth pointing out that the studied numerical case is an unsteady problem, for brevity but without loss of generality, only the simulation results obtained at $t = 13.5$ days are presented.

Figure 7 shows the comparison of reconstruction accuracy of POD-DEIM-ROM (red solid line) and standard FDM (blue dashed line) in this case. It can be clearly seen that in the four figures the red solid line and blue dashed line agree well with each other, which indicates the pressure, compressibility factor and Darcy velocity of the natural gas flow can all be reconstructed accurately by the POD-DEIM-ROM. Compared with the traditional FDM under the same calculation conditions, the deviation between these two lines is not noticeable and can be neglected. Thus in this case, numerical results obtained by POD-DEIM-ROM match well with those obtained by FDM, the proposed POD-DEIM-ROM demonstrates excellent reconstruction accuracy.

Figure 7: Comparison of reconstruction accuracy of POD-DEIM-ROM (red solid line) and FDM (blue dashed line) in numerical case 1

To validate the reconstruction accuracy of POD-DEIM-ROM quantitatively, the below defined average relative errors between reconstructed pressure, Darcy velocity and compressibility factor by POD-DEIM-ROM and those calculated by FDM are presented in Table 4.

$$\varepsilon_M = \frac{\sum_{i=1}^{nx} \sum_{j=1}^{ny} \left| \frac{M_1 - M_2}{M_2} \right|}{nx \times ny} \times 100\% \quad (21)$$

where ε_M denotes the average relative error; M denotes p, u, v, Z , respectively; M_1 denotes the results computed by POD-DEIM; M_2 denotes the results computed by FDM; nx and ny denote the grid number along x and y directions.

From Table 4, it can be found that the pressure and compressibility factor have an excellent reconstruction accuracy, especially the average relative error of compressibility factor is only 0.0026%. It is obvious to observe the average relative error of Darcy velocity is larger than those of pressure and compressibility factor, the main reason can be clarified by Equation (2) that the relative error of Darcy velocity is influenced by both the permeability of porous media and fluid viscosity. Overall, the average relative errors can verify that the proposed POD-DEIM-ROM possesses excellent computational performance from the perspective of reconstruction accuracy in this case.

Table 4: Average relative errors between the results reconstructed by POD-DEIM-ROM and calculated by FDM in numerical case 1

Variable	Average relative error
p	0.089%
u	0.363%
v	0.125%
Z	0.0026%

Except for the reconstruction accuracy, the computational speed-up of POD-DEIM-ROM is much more concerned, which is the main aim of this work. Therefore, the CPU time of POD-DEIM-ROM and FDM consumed in the simulation is recorded and analyzed in detail, as shown in Figure 8. In this figure, the left part represents the CPU time of FDM and the right part represents the CPU time of POD-DEIM-ROM consumed for simulating 13.5 days. The black bar is the total CPU time consumed in this case, the red bar represents the CPU time used to solve the pressure equation, and the blue bar represents the CPU time consumed to solve the P-R EOS. It can be seen from the comparison that in FDM 97.4% of the CPU time was consumed to solve the P-R EOS, however, in POD-DEIM-ROM the corresponding CPU time was decreased substantially to a very small value, 15.3%. Overall, the absolute CPU time of POD-DEIM-ROM was largely decreased compared with that of FDM, and the speed-up ratio of POD-DEIM-ROM to FDM is up to 58.4. It indicates that the proposed POD-DEIM-ROM is an efficient acceleration approach that can largely improve the numerical efficiency of the traditional FDM. Moreover, Figure 8 also proves that DEIM-ROM is an perfect choice to solve the P-R EOS, the speed-up ratio of DEIM-ROM for solving the P-R EOS is up to 371 compared with that of FDM. To the best of authors' knowledge, there is no report on the solution of P-R EOS using DEIM approach. For the pressure equation, the calculation time is also reduced when using the POD-ROM, but the acceleration is not obvious compared with the DEIM-ROM. The main reason can be explained from the aspect that in this case the pressure equation part can be easier solved, and the convergence criterion for iterative solution of pressure is not so strict, thus the computational speed-up for solving the pressure equation is not obvious. Overall, the efficient solving of P-R EOS contributes most of the computational saving in this case, the computational speed up of POD-DEIM-ROM is very attractive, which is two orders of magnitude faster than the traditional FDM.

Figure 8: Comparison of CPU time of POD-DEIM-ROM and FDM in numerical case 1

As mentioned before, the selection of POD modes and DEIM interpolation points can exert significant impacts on numerical accuracy and speed-up of POD-DIM-ROM. To investigate those influences induced by POD modes and DEIM interpolation points selection, here the average relative errors of pressure, Darcy velocity and compressibility factor with different POD mode numbers and DEIM

interpolation point numbers are presented in Figure 9, the profile of speed-up ratio with different POD mode numbers and DEIM interpolation point numbers is shown too in Figure 9. From Figures 9a ~9c, it can be seen that POD modes number has critical effects on the computational accuracy of POD-DEIM-ROM. With the increase of POD modes number, the average relative errors of pressure, Darcy velocity and compressibility factor all decrease, but this trend would be reduced slowly when enough POD modes are adopted. Compared with the effect of POD modes number, the selection of DEIM interpolation points demonstrates slight influences on accuracy of pressure and Darcy velocity, it is hard to find any distinctions in the average relative errors of pressure and Darcy velocity when different DEIM interpolation points are selected. However, Figure 9c indicates that the selection of DEIM interpolation points affects the accuracy of compressibility factor substantially, generally the increasing interpolation points lead to decreasing average relative errors. It also implies that in this numerical case 10 interpolation points are enough to capture the compressibility factor, more extra points have no contribution to the calculation accuracy even sometimes exert negative effects. From Figure 9d, it is obvious to find that with the rise of POD modes number and DEIM interpolation points number, the computational speed-up would decline almost linearly. The effect of POD modes number on the acceleration overweighs that of DEIM interpolation points. It is also interesting to see that when POD modes number and DEIM interpolation points are larger enough, the influence of interpolation points number on speed-up will be submerged. Figure 9 also proofs that our selection of POD modes and DEIM interpolation points in subsection 5.1.1 is reasonable. In conclusion, the selection of POD modes and DEIM interpolation points should be implemented carefully, trade-offs between accuracy and speed-up should be considered.

Figure 9: Influence of POD modes and DEIM interpolation points numbers on accuracy and speed-up in numerical case 1

5.2. Numerical case 2

In this case, the predictability of POD-DEIM-ROM is validated and demonstrated with different boundary values at offline stage and online stage. The permeability distribution of computational domain is shown in Figure 10 where the two blue bars denote low permeable regions, and the boundary type is same as that in numerical case 1. Detailed calculation parameters are presented in Table 5.

Figure 10: Permeability distribution in numerical case 2

Table 5: Calculation parameters in numerical case 2

Parameter	Value	Parameter	Value
ϕ	0.2	W	$1.6 \times 10^{-2} \text{ kg / mol}$
p_0	$1.01325 \times 10^5 \text{ Pa}$	μ	$1.5 \times 10^{-4} \text{ Pa} \cdot \text{s}$
p_1	$4.053 \times 10^5 \text{ Pa}$	$lx \times ly$	$100 \text{ m} \times 50 \text{ m}$
p_2	$1.01325 \times 10^5 \text{ Pa}$	$nx \times ny$	100×50
k_1	$1.5 \times 10^{-1} \text{ D}$	T_b	111.63 K
k_2	$1.0 \times 10^{-2} \text{ D}$	T_c	190.58 K
R	$8.314 \text{ J / (mol.k)}$	T	285.87 K
q	0	p_c	$4.604 \times 10^6 \text{ Pa}$
Δt	$3.0 \times 10^{-4} \text{ day}$	simulation time	30 days

At the offline stage, the representative pressure samples and $f(Z)$ samples are calculated with four groups of pressure setting where p_1 is set as 3.03975×10^5 Pa and 4.053×10^5 Pa, p_2 is set as 1.519875×10^5 Pa and 2.533125×10^5 Pa, respectively. 500 samples in each group are considered thus totally 2000 samples are obtained respectively for pressure and $f(Z)$. Readers of interest can refer to [19] for more details on how to get representative samples.

5.2.1. Determination of POD modes and DEIM interpolation points

Just as numerical case 1, first the number of POD modes and DEIM interpolation points should be determined. Using the same approach presented in subsection 5.1.1, in this case 10 POD modes and 10 DEIM interpolation points are selected too. Figure 11 illustrates locations of the selected 10 interpolation points.

Figure 11: Selected interpolation points in DEIM-ROM, the indexes of these points are: (100, 50), (8, 1), (28, 32), (1, 50), (43, 1), (22, 1), (25, 41), (72, 14), (15, 37), (33, 50)

5.2.2. Results discussion

In this part, the prediction accuracy and computational speed-up of proposed POD-DEIM-ROM are evaluated and compared with those of FDM in detail. Figure 12 shows the pressure distribution predicted by POD-DEIM-ROM (red solid line) and standard FDM (blue dashed line) at $t = 30$ days. It can be found that the result of POD-DEIM-ROM matches well with the FDM result, the two lines almost overlap with each other and the distinction between these two lines is negligible. Therefore, the POD-DEIM-ROM is able to predict the pressure accurately. In Figure 13, the comparison of Darcy velocity computed by POD-DEIM-ROM and FDM is presented. Although the deviation of these two simulation results at some specific locations is much larger than that of pressure, the overall results of POD-DEIM-ROM are still in good agreement with those of FDM. The reason for the larger error of Darcy velocities compared with pressure is mainly attributing to the sensitive relations between the pressure and Darcy velocity. According to Darcy's law, a small variation of pressure can lead to a large change of Darcy velocity if the hydraulic coefficient (ratio of permeability to dynamic viscosity) is relatively large. Figure 14 demonstrates the comparison of compressibility factor computed by POD-DEIM-ROM and FDM. It is observed that calculation results of compressibility factor using these two approaches almost overlap with each other, which indicates the proposed POD-DEIM-ROM possesses a satisfactory prediction accuracy.

Figure 12: Comparison of pressures predicted by POD-DEIM-ROM (red solid line) and FDM (blue dashed line) in numerical case 2

Figure 13: Comparison of Darcy velocity predicted by POD-DEIM-ROM (red solid line) and FDM (blue dashed line) in numerical case 2

Figure 14: Comparison of compressibility factor predicted by POD-DEIM-ROM (red solid line) and FDM (blue dashed line) in numerical case 2

In Table 6, the average relative errors of predicted pressure, Darcy velocity and compressibility factor are presented to validate the prediction ability of POD-DEIM-ROM quantitatively. From Table 6 it can be seen the pressure and compressibility factor have an excellent prediction accuracy with the errors as small as 0.330% and 0.003%, respectively. The average relative error of Darcy velocity is larger than that of pressure and compressibility factor, but it still be acceptable from the perspective of engineering. On the whole, the average relative errors of quality of interest in this case can fully demonstrate that the proposed POD-DEIM-ROM is capable of predicting the model problem accurately.

Table 6: Average relative errors between the results predicted by POD-DEIM-ROM and calculated by FDM in numerical case 2

Variables	Average relative error
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p	0.330%
u	7.097%
v	3.045%
Z	0.003%

Figure 15 shows the CPU time of POD-DEIM-ROM and FDM consumed in numerical simulation of case 2. It can be observed that 98.7% of the CPU time in FDM was consumed to solve the P-R EOS, which indicates that the P-R EOS is the main challenge for the efficient solution of compressible porous gas flow. By using DEIM-ROM, the corresponding CPU time used to solve P-R EOS was decreased to 16.7s, only 19.9% of the total CPU time, and the computational efficiency of DEIM solving P-R EOS is as high as 359.2 times of FDM. The absolute CPU time of POD-DEIM-ROM was largely decreased compared with FDM (from 6076.8s to 84.1s), and the speed-up ratio of POD-DEIM-ROM to FDM is up to 72. It indicates that the DEIM-ROM is an efficient approach and excellent choice to solve the P-R EOS. Again, the attractive advantage of POD-DEIM-ROM is well illustrated from the perspective of computational efficiency, which is vital for engineering applications in the development of natural gas reservoirs.

Figure 15: Comparison of CPU time of POD-DEIM-ROM and FDM in numerical case 2

6. Conclusions

In this study, a hybrid reduced order model coupling the POD and DEIM approaches is presented to accelerate the simulations of single-phase compressible gas flow in porous media, which is highly demanded in petroleum engineering. The establishment of POD-DEIM-ROM is introduced in detail, and the key point of POD-DEIM-ROM that how to select POD modes and DEIM interpolation points is demonstrated. The numerical performances including the reconstruction and prediction accuracy and computational speed-up of proposed POD-DEIM-ROM are validated through two numerical cases. The main concluding remarks of this work can be summarized as follows,

- (1) A POD-DEIM-ROM is established in this study for fast calculation of compressible natural gas flow in porous media considering the Peng-Robinson EOS, in which the POD-ROM is used to solve the pressure equation and the DEIM-ROM is applied to solve the Peng-Robinson EOS, respectively. By using these two reduced order models, the original full order problem can be solved efficiently in a low dimensional space with small degrees of freedom.
- (2) The determination of POD modes and DEIM interpolation points has appreciable effects on the prediction accuracy and computational speed-up of POD-DEIM-ROM, overall the influence of POD modes number overweighs that of DEIM interpolation points. Therefore, trade-offs between numerical accuracy and computational acceleration should be considered carefully when selecting the POD modes and DEIM interpolation points.
- (3) The reconstructed and predicted results of proposed POD-DEIM-ROM match well with those of standard finite difference method, especially the pressure and compressibility factor. It indicates that the POD-DEIM-ROM possesses satisfactory prediction accuracy. Compared with FDM, the computational speed-up of POD-DEIM-ROM is attractive, generally the simulation using POD-DEIM-ROM is approximate two orders of magnitude faster than that using FDM.

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