

Original article

Adaptive time-splitting scheme for two-phase flow in heterogeneous porous media

Mohamed F. El-Amin^{1,2*}, Jisheng Kou³, Shuyu Sun², Amgad Salama⁴

¹College of Engineering, Effat University, Jeddah 21478, Kingdom of Saudi Arabia

²Computational Transport Phenomena Laboratory (CTPL), Division of Physical Sciences and Engineering (PSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Kingdom of Saudi Arabia

³School of Mathematics and Statistics, Hubei Engineering University, Xiaogan 432000, P. R. China

⁴Process System Engineering, Produced Water Treatment Laboratory, Faculty of Engineering, University of Regina, Regina, SK, Canada

(Received November 20, 2017; revised December 3, 2017; accepted December 5, 2017; published December 25, 2017)

Abstract: In the present paper, an adaptive time-splitting scheme is introduced to investigate the problem of two-phase flow in heterogeneous porous media. The pressure and saturation equations are coupled by the capillary pressure which is linearized in terms of saturation. An Implicit Pressure Explicit Saturation scheme is used to solve the problem under consideration. We use the time schemes for the pressure and saturation equations. The external time interval is divided into two levels, the first level is for the pressure, the second one is for the saturation. This method can reduce the computational cost arisen from the implicit solution of the pressure equation and the rapid changes in saturation. The time-step size for saturation equation is adaptive under computing and satisfying the Courant–Friedrichs–Lewy (CFL<1) condition. In order to show the well performance of the suggested scheme, we introduce a numerical example of a highly heterogeneous porous medium. The adaptive time step-size is shown in graphs as well as the water saturation is shown in contours.

Keywords: Time-splitting, IMPES, two-phase flow, porous media, reservoir simulation.

Citation: El-Amin, M., Kou, J., Sun, S., et al. Adaptive time-splitting scheme for two-phase flow in heterogeneous porous media. *Adv. Geo-Energy Res.* 2017, 1(3): 182-189, doi: 10.26804/ager.2017.03.05.

1. Introduction

The Implicit Pressure Explicit Saturation (IMPES), is a conditionally stable approach, solves the pressure equation implicitly and updates the saturation explicitly. Hence it takes very small time step size, in particular with heterogeneous porous media. The IMPES scheme has been improved in several versions (Young and Stephenson, 1983; Lu, 2000; Coats, 2001; Chen et al., 2006; Kou and Sun, 2010). The temporal discretization scheme is considered an important factor that affect efficiency of numerical reservoir simulators. The application of traditional single-scale temporal scheme is restricted by the rapid changes of the pressure and saturation with capillarity and concentrations if applicable. So, applying time splitting strategies has a significant improvement to treating the gap between the pressure and the saturation.

Time splitting method has been considered in a number of publications (Smolinski et al., 1988; Belytschko and Lu, 1993; Singh and Bhallamudi, 1996; Smolinski et al., 1996; Singh and Bhallamudi, 1997; Gravouil and Combescure, 2000; Klisinski, 2001; Bhallamudi et al., 2003; Park et al., 2008; Sun and Geiser, 2008; Wang et al., 2012; Wang et al., 2017). For example, in (Singh and Bhallamudi, 1996; Singh and Bhallamudi, 1997), an explicit subtiming scheme is provided. On the other hand, an implicit time-stepping schemes have been proposed by Bhallamudi et al. (2003). Similar methodology has been used to the problem of flow and transport simulations in fractured porous media (Park et al., 2008). VanderKwaak (1999) have introduced a hybrid implicit-explicit scheme by treating implicitly some portions of the domain under certain stability conditions, while the rest of the domain is treated by the

*Correspondent author. Email: mohamed.elamin.kaust@gamil.com

explicit time-stepping approach. Kou et al. (2011) have developed a multiscale time-splitting strategy for simulating two-phase flow in fractured porous media. In El-Amin et al. (2016) we have introduced nonlinear iterative IMPES-IMC (IMPLICIT Pressure Explicit Saturation-IMPLICIT Concentration) scheme to solve the flow equation of the model of nanoparticles transport in porous media. Recently, El-Amin et al. (2017a) presented a convergence analysis of the nonlinear iterative IMPES-IMC method for a two-phase flow in porous media associated with nanoparticle injection. The authors (El-Amin et al., 2017b) have investigated the problem of nanoparticles transport in fractured porous media, numerically using a multi-scale time-splitting strategy. Also, they (El-Amin et al., 2017c) have introduced a multi-scale adaptive time-splitting technique for nonisothermal two-phase flow and nanoparticles transport in heterogeneous porous media. Recently, the discrete-fracture model (DFM) of two-phase immiscible incompressible flow including nanoparticles transport in fractured heterogeneous porous media has been studied (El-Amin et al., 2017d).

This work is devoted to a time-stepping technique for the modeling and simulation two-phase flow in porous media. The IMPES scheme is employed to solve the problem under consideration, and the CCFD method is used for the spatial discretization. The time-stepping scheme is applied under the CFL condition to adapting the time-steps sizes. Finally, numerical experiments are provided. The paper is organized as follows: The second section is devoted for the modeling and mathematical formulation. The third section is devoted to the time-stepping technique. The time-steps adaption is provided in the fourth section. The CCFD spatial discretization is introduced in Section 5. Then, Section 6 is devoted for numerical tests, while the conclusions was presented in Section 7.

2. Modeling and mathematical formulation

This paper considers the problem of two-phase immiscible incompressible flow in porous media. The governing equations consists of water saturation and Darcy's law. In the following we introduce the governing equations briefly:

$$\mathbf{u}_\alpha = -\frac{k_\alpha}{\mu_\alpha} \nabla \Phi_\alpha, \quad \alpha = w, n \quad (1)$$

$$k_\alpha = k_{r\alpha} \mathbf{K}, \quad \Phi_\alpha = p_\alpha + \rho_\alpha g \nabla z, \quad \alpha = w, n$$

$$\phi \frac{\partial s_\alpha}{\partial t} + \nabla \cdot \mathbf{u}_\alpha = q_\alpha, \quad \alpha = w, n \quad (2)$$

$$s_w + s_n = 1$$

where \mathbf{K} is the permeability tensor $\mathbf{K} = k\mathbf{I}$, where \mathbf{I} is the identity matrix and k is a positive real number. ϕ is the porosity, g is the gravitational acceleration, and z is the depth. $\mathbf{u}_\alpha, \Phi_\alpha, p_\alpha, \mu_\alpha, \rho_\alpha, k_\alpha, k_{r\alpha}, q_\alpha, s_\alpha$ are, respectively, the velocity, the pressure potential, the pressure, the viscosity, the density, the effective permeability, the relative permeability, the external mass flow rate, and the saturation of the phase α . w stands for the wetting phase (water), and n stands for the nonwetting phase (oil).

Providing the following definitions:

The capillary pressure: $p_c(s_w) = p_n - p_w$.

The total velocity: $\mathbf{u}_t = \mathbf{u}_w + \mathbf{u}_n$.

The flow fraction: $f_w = \lambda_w / \lambda_t$.

The phase mobility: $\lambda_\alpha = k_{r\alpha} / \mu_\alpha$.

The total mobility: λ_t .

The capillary pressure potential: $\Phi_c = (\rho_n - \rho_w) g \nabla z + p_c$.

The total source mass transfer: $q_t = q_w + q_n$.

After some mathematical manipulations and referring to Hoteit and Firoozabadi (2008), the pressure equation can be rewritten as,

$$\nabla \cdot \mathbf{u}_t = -\nabla \cdot \lambda_t \mathbf{K} \nabla \Phi_w - \nabla \cdot \lambda_n \mathbf{K} \nabla \Phi_c = q_t \quad (3)$$

Because this equation contents the capillary pressure which is a function of saturation, it will be coupled with the following saturation equation to calculate the pressure:

$$\phi \frac{\partial s_w}{\partial t} - q_w = -\nabla \cdot \lambda_w \mathbf{K} \nabla \Phi_w \quad (4)$$

However, the saturation is updated using the following form,

$$\phi \frac{\partial s_w}{\partial t} - q_w = -\nabla \cdot (f_w \mathbf{u}_a) \quad (5)$$

where $\mathbf{u}_w = f_w \mathbf{u}_a$ and $\mathbf{u}_a = -\lambda_t \mathbf{K} \nabla \Phi_w$.

In this study, given the the normalized wetting phase saturation,

$$S = \frac{s_w - s_{wr}}{1 - s_{nr} - s_{wr}}, \quad 0 \leq S \leq 1$$

the capillary pressure is defined as,

$$p_c = -p_e \log S$$

and the relative permeabilities are defined as,

$$k_{rw} = k_{rw}^0 S^2, \quad k_{rn} = k_{rn}^0 (1 - S)^2$$

where

$$k_{rw}^0 = k_{rw}(S = 1), \quad k_{rn}^0 = k_{rn}(S = 1)$$

where p_e is the capillary pressure parameter, s_{wr} is the irreducible water saturation and s_{nr} is the residual oil saturation after water flooding.

Consider the computational domain Ω with the boundary $\partial\Omega$ which is subjected to Dirichlet Γ_D and Neumann Γ_N boundaries, where $\partial\Omega = \Gamma_D \cup \Gamma_N$ and $\Gamma_D \cap \Gamma_N = \emptyset$. At the beginning of the injection process, we have,

$$s_w = s_w^0, \quad \text{in } \Omega \quad \text{at } t = 0 \quad (6)$$

The boundary conditions are given as,

$$p_w \text{ (or } p_n) = p^D \quad \text{on } \Gamma_D \quad (7)$$

$$\mathbf{u}_t \cdot \mathbf{n} = q^N, \quad s_w = S^N, \quad \text{on } \Gamma_N \quad (8)$$

Table 1. Values of the physical parameters.

Parameter	Value	Units
S_{wr}	0.001	–
S_{nr}	0.001	–
ϕ	0.3	–
μ_w	1	cP = 1.0×10^{-3} Pa · s
μ_n	0.45	cP
k_{rw0}	1	–
k_{ro0}	1	–
B_c	50	bar = 1.0×10^5 Pa
Total grid-cells	6000	–
Outer loop, k	50, 100, 200	–

where \mathbf{n} is the outward unit normal vector to $\partial\Omega$, p^D is the pressure on Γ_D and q^N the imposed inflow rate on Γ_N , respectively.

3. Adaptive time-splitting method

In the time splitting method, the pressure is coupled with the saturation in each time-step. The time-step size for the pressure can be taken larger than the one of saturation. The total time interval of the pressure, $[0, T]$ is divided into N_p , time-steps as $0 = t_0 < t_1 < \dots < t_{N_p} = T$. Thus, the time-step length assigned for the pressure is, $\Delta t^k = t^{k+1} - t^k$. On the other hand, as the saturation varies more rapidly than the pressure, we use a smaller time-step size for the saturation equation. That is, each interval, $(t^k, t^{k+1}]$, will be divided into $N_{p,s}$ subintervals as $(t^k, t^{k+1}] = \cup_{l=0}^{N_{p,s}-1} (t^{k,l}, t^{k,l+1}]$. Therefore, the governing equations, Eq. (3) and (4) are solved based on the adaptive time-splitting technique. The capillary pressure function, Φ_c is linearized in terms of the saturation using the following formula,

$$\Phi_c(s_w^*) \cong \Phi_c(s_w^k) + \Phi_c'(s_w^k) [s_w^{k+1} - s_w^k] \quad (9)$$

where Φ_c' is derivative of Φ_c . The quantity, $[s_w^{k+1} - s_w^k]$, can be calculated from the saturation equation,

$$s_w^{k+1} - s_w^k = \frac{\Delta t^k}{\phi} \left[q_w^{k+1} - \nabla \cdot \lambda_r(s_w^k) \mathbf{K} \nabla \Phi_w^{k+1} \right] \quad (10)$$

In addition to the pressure equation,

$$-\nabla \cdot \lambda_r(s_w^k) \mathbf{K} \nabla \Phi_w^{k+1} - \nabla \cdot \lambda_n(s_w^k) \mathbf{K} \nabla \Phi_c(s_w^*) = q_t^{k+1} \quad (11)$$

Then, the above coupled Eq. (9), (10) and (11) is solved implicitly to obtain the pressure potential. Therefore, the saturation is updated explicitly with using the upwind scheme for the convection term as,

$$\phi \frac{s_w^{k,l+1} - s_w^{k,l}}{\Delta t^l} + \nabla \cdot (f_w^k \mathbf{u}_a^{k+1}) = q_w^{k,l+1} \quad (12)$$

In the proposed algorithm, we check if the CFL condition is satisfying, namely, $\text{CFL} < 1$. The CFL may be defined as follows,

$$\text{CFL}_x = \frac{\mathbf{u}_x \Delta t^{k,l}}{\Delta x} \quad (13)$$

and

$$\text{CFL}_y = \frac{\mathbf{u}_y \Delta t^{k,l}}{\Delta y} \quad (14)$$

for saturation equation. It is know that the CFL depends on the ratio $\Delta t / \Delta x$ which can be fixed at larger time-steps and larger mesh-size. Thus, when we use a larger domain (larger mesh size) then we can use larger time step size. In the implementation, the initial time-step for the saturation equation is taken as the pressure time-step, i.e., $\Delta t^{k,0} = \Delta t^k$, and the initial time-step for the concentration equation is taken as the saturation time-step, i.e., $\Delta t^{k,l,0} = \Delta t^{k,l}$. Then, we check if $\text{CFL}_x > 1$ or $\text{CFL}_y > 1$, the saturation time-step will be divided by 2 and the CFL_x and CFL_y will be recalculated. This procedure will be repeated until satisfying the condition $\text{CFL}_x < 1$ and $\text{CFL}_y < 1$, then the final adaptive saturation time-step will be obtained.

4. Spatial discretization

The cell-centered finite difference (CCFD) is a locally conservative method that is very useful in solving petroleum reservoir simulation problems. Arbogast et al. (1997) have proved that the CCFD method is equivalent to the mixed finite element method in the case of rectangular elements. In this work, we apply the CCFD scheme to the system of Eqs. (9)-(12). The corresponding algebraic coupled pressure and saturation equation are solved implicitly to obtain the pressure is given as,

$$\mathbf{A}_t(s_w^k) \mathbf{m}_w^{k+1} = \mathbf{Q}_t(s_w^k) \quad (15)$$

where

$$\mathbf{A}_t(s_w^k) = \mathbf{A}_a(s_w^k) - \Delta t^l \mathbf{A}_c(s_w^k) \mathbf{m}'(s_w^k) \mathbf{M}^{-1} \mathbf{A}_w(s_w^k) \quad (16)$$

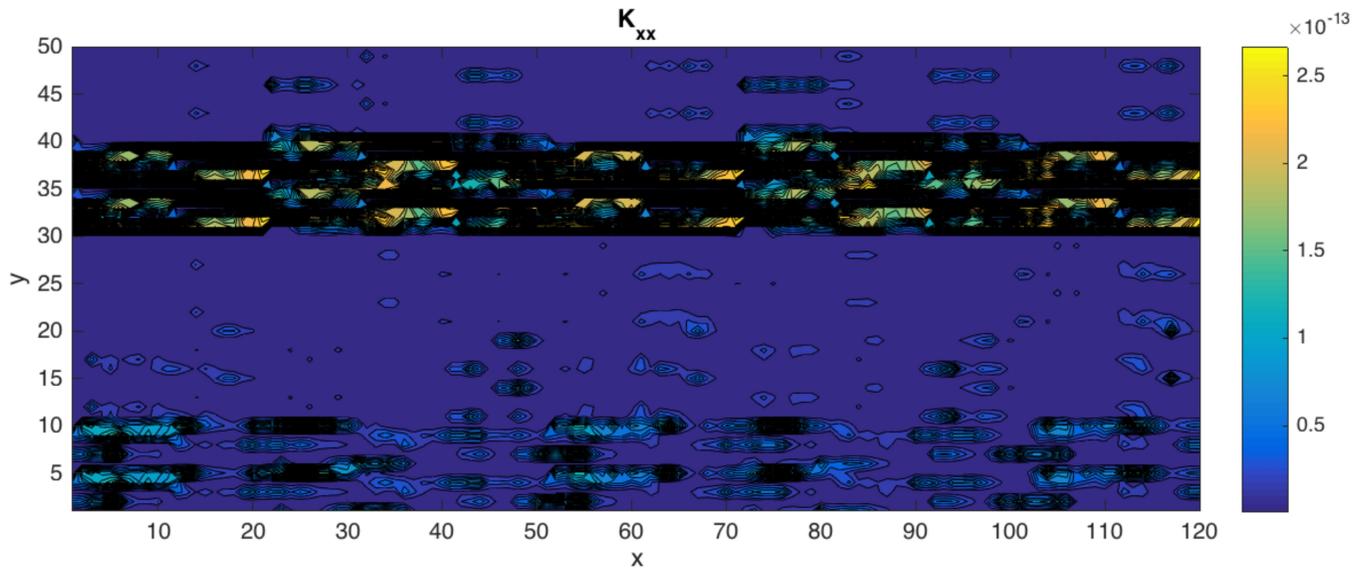


Fig. 1. Real heterogenous permeability map.

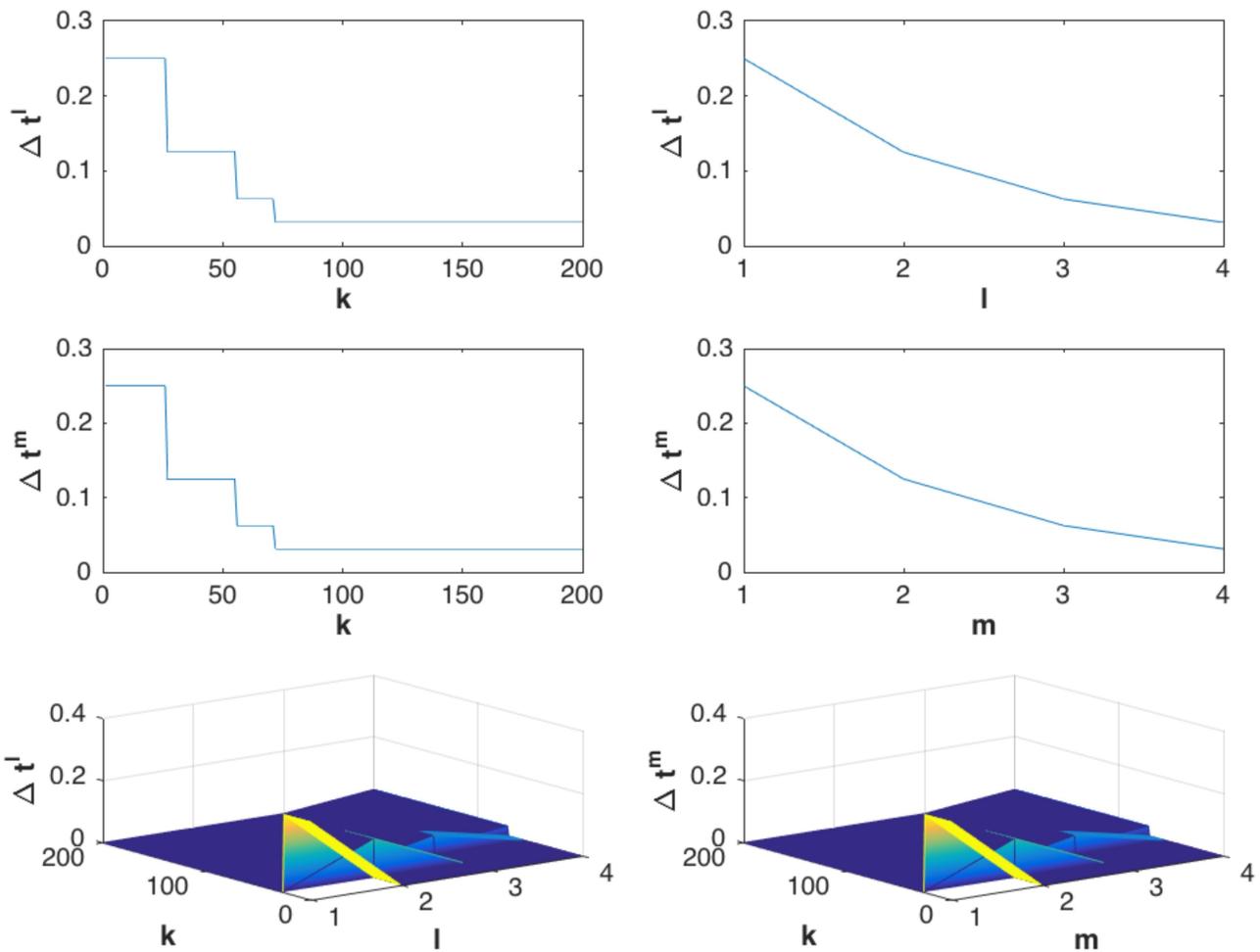


Fig. 2. Adaptive time-step size, Δt^l against the number of steps of the outer loop k and the number of the inner loops l at $k = 200$.

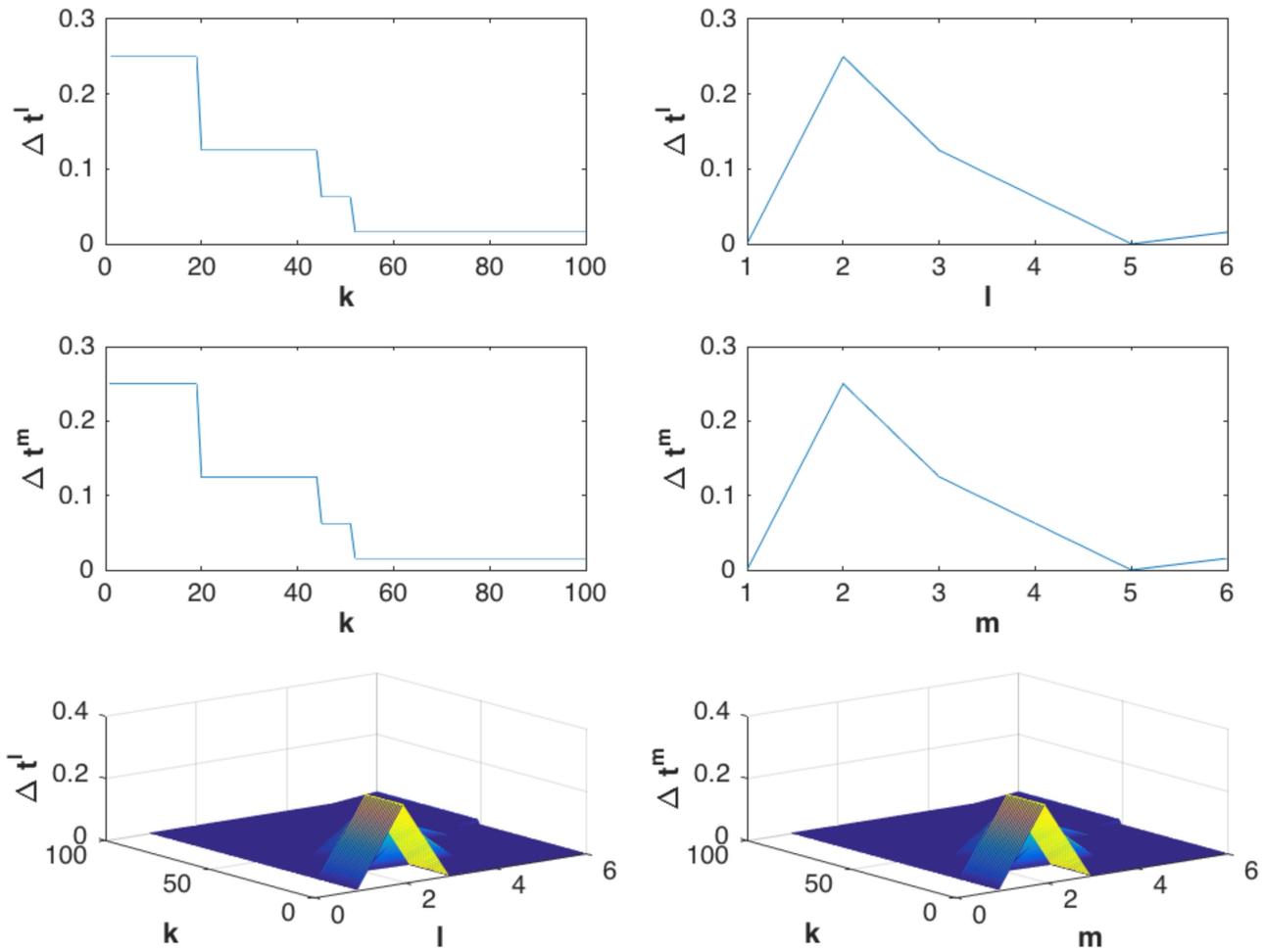


Fig. 3. Adaptive time-step sizes, Δt^l and Δt^m against the number of steps of the outer loop k and the number of the inner loops l and m : Case 2 ($\Delta t^k = 100$).

and,

$$\begin{aligned} \mathbf{Q}_t(\mathbf{s}_w^k) = & \mathbf{Q}_{ac}^{k+1} - \mathbf{A}_c(\mathbf{s}_w^k) [\mathbf{m}_c(\mathbf{s}_w^k) + \mathbf{m}'(\mathbf{s}_w^k) (\mathbf{s}_w^k - \mathbf{s}_w^{k+1})] \\ & - \Delta t^l \mathbf{A}_c(\mathbf{s}_w^k) \mathbf{m}'(\mathbf{s}_w^k) \mathbf{M}^{-1} \mathbf{Q}_w^{k+1} \end{aligned} \quad (17)$$

After calculating the pressure and the velocity, the CCFD scheme of Eq. (12) to update the saturation is the following algebraic equation,

$$\mathbf{M} \frac{\mathbf{s}_w^{k,l+1} - \mathbf{s}_w^k}{\Delta t^l} + \mathbf{A}_s(\mathbf{u}_a^{k+1}) f_w(\mathbf{s}_w^k) = \mathbf{Q}_s^{k,l+1} \quad (18)$$

5. Numerical tests

In order to examine the performance of the current scheme we introduce some numerical examples in this section. Firstly, we introduce the required physical parameters used in the computations. Then, we study the performance of the scheme by introducing some results for the adaptive time steps based on values of the corresponding CFL. Then we present some

results for the distributions of water saturation. The values and units of the physical parameters are inserted in Table 1.

In this study, we use a real permeability map of dimensions 120×50 , which is vary in a large scope and highly heterogenous (Al-Dhafeeri and Nasr-El-Din, 2007) (see the permeability map, Fig. 1). We consider a domain of size $40 \text{ m} \times 16 \text{ m} \times 1 \text{ m}$ which is discretized into 120×50 uniform rectangles grids. The injection rate was 0.01 Pore-Volume-Injection (PVI) and continued the calculation until 0.5 PV. In this example, we choose the number of steps of the outer loop to be $k = 200$ (see Fig. 2). In this figure, the adaptive time-step size, Δt^l is plotted against the number of steps of the outer loop k and the number of the inner loops l . It can be seen from this figure that Δt^l starts with large values then they gradually become smaller and smaller as k increases. On the other hand, one may note that Δt^l starts with large values then they gradually becomes smaller and smaller as l increases. Moreover, Fig. 3 illustrates adaptive time-step size, Δt^l against the number of steps of the outer loop k and the number of the inner loops l at $k = 100$. Finally, Fig. 4 adaptive time-step sizes, Δt^l and Δt^m against the number of steps of the outer loop k and the number of the inner loops l and m ($\Delta t^k = 50$).

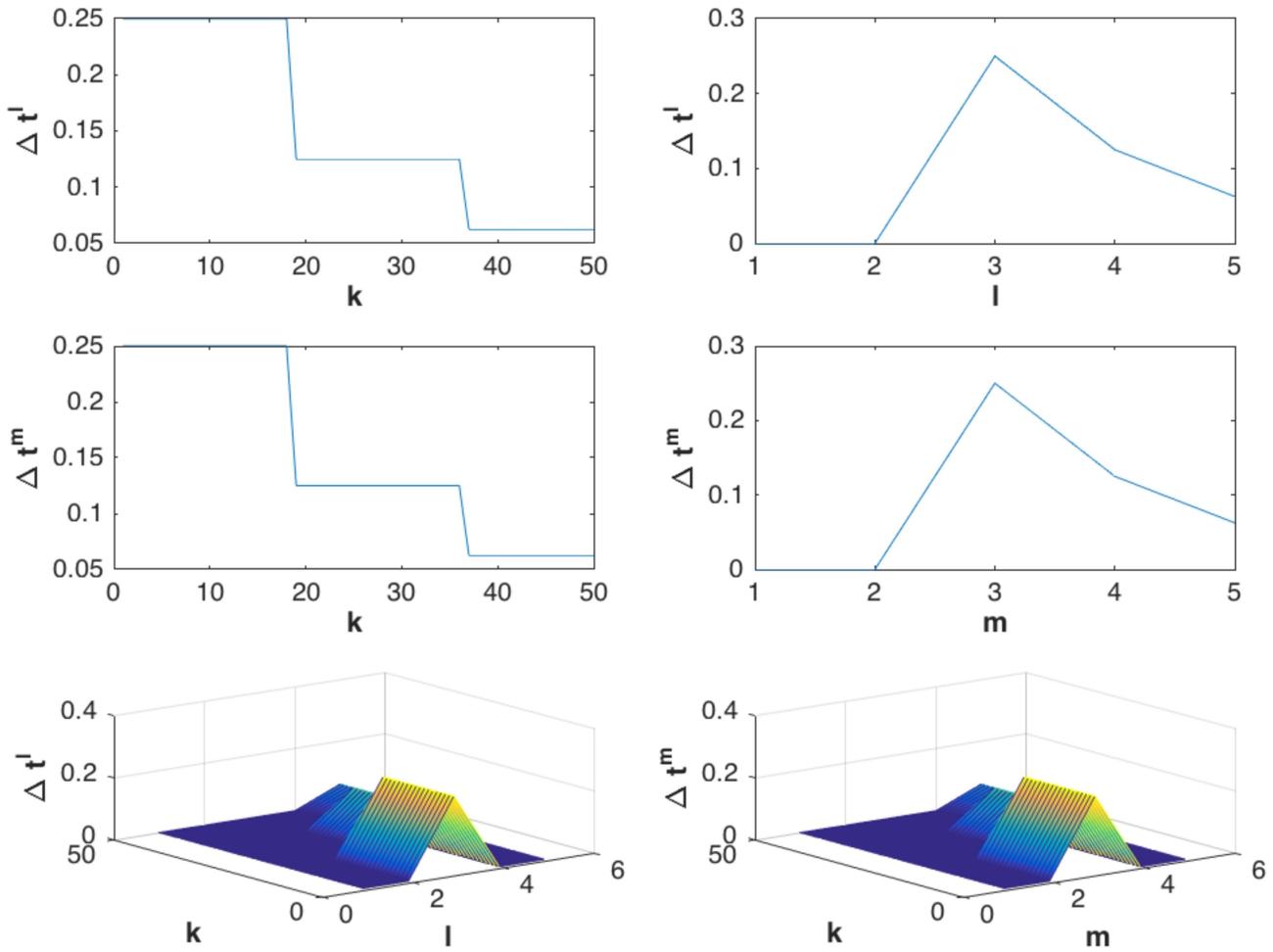


Fig. 4. Adaptive time-step sizes, Δt^l and Δt^m against the number of steps of the outer loop k and the number of the inner loops l and m : Case 1 ($\Delta t^k = 50$).

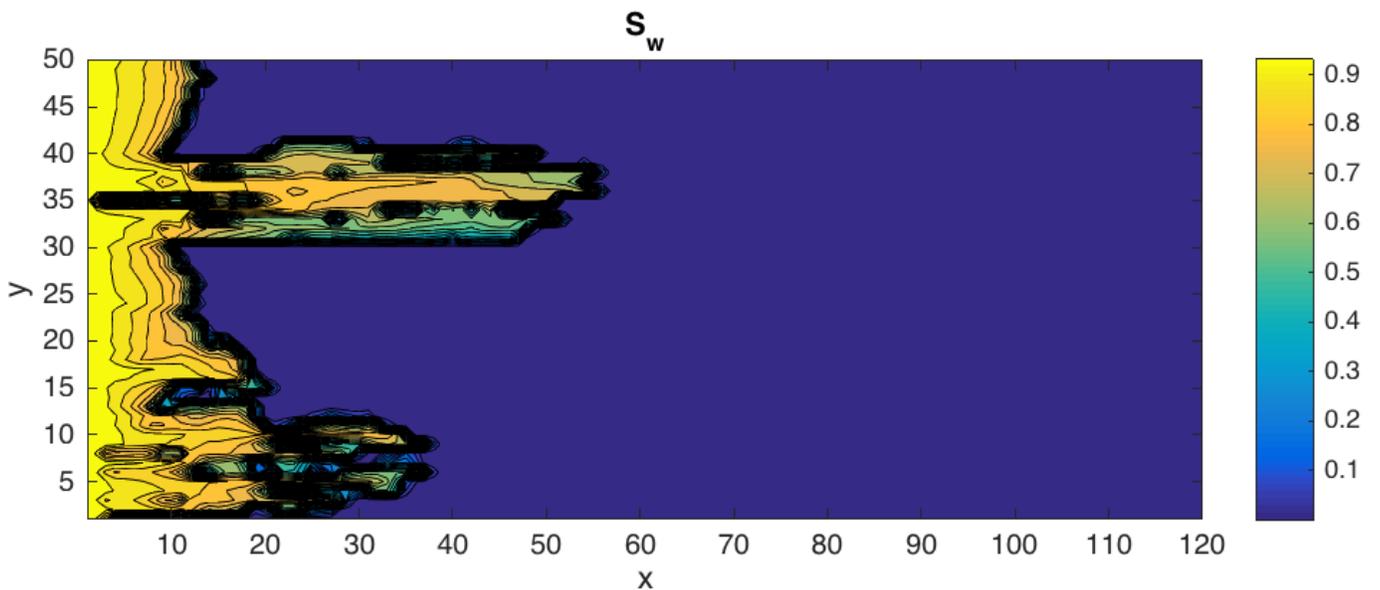


Fig. 5. Distribution of water saturation at 0.15 PV.

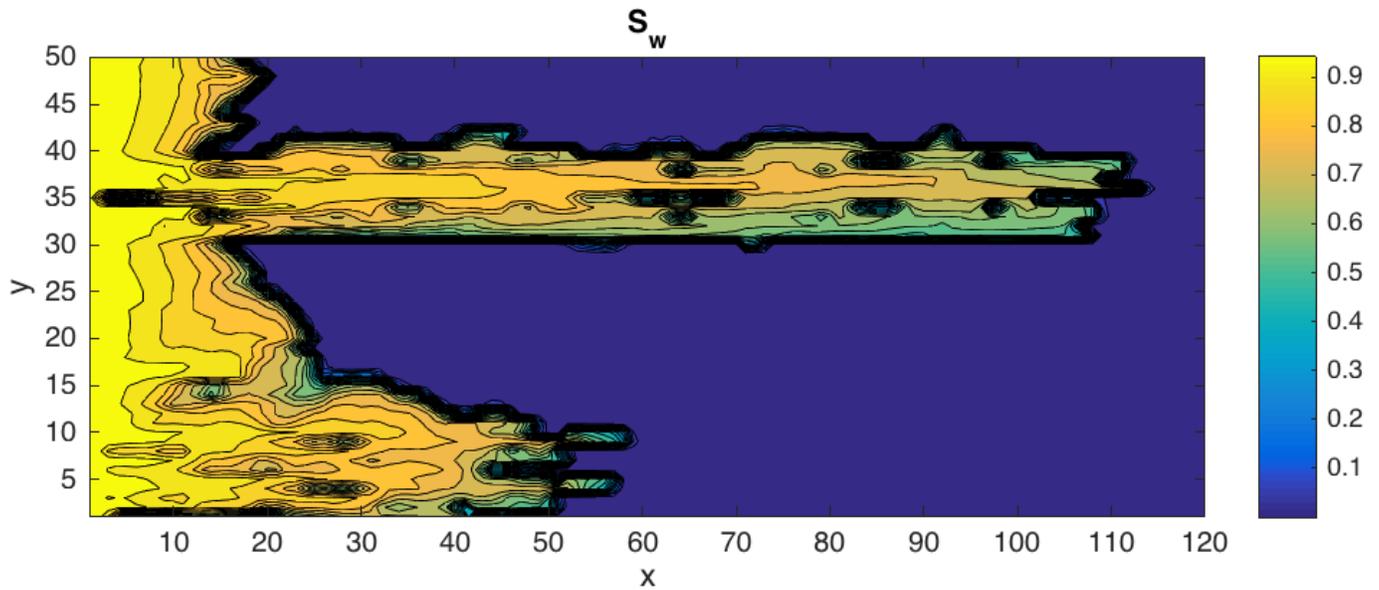


Fig. 6. Distribution of water saturation at 0.3 PV.

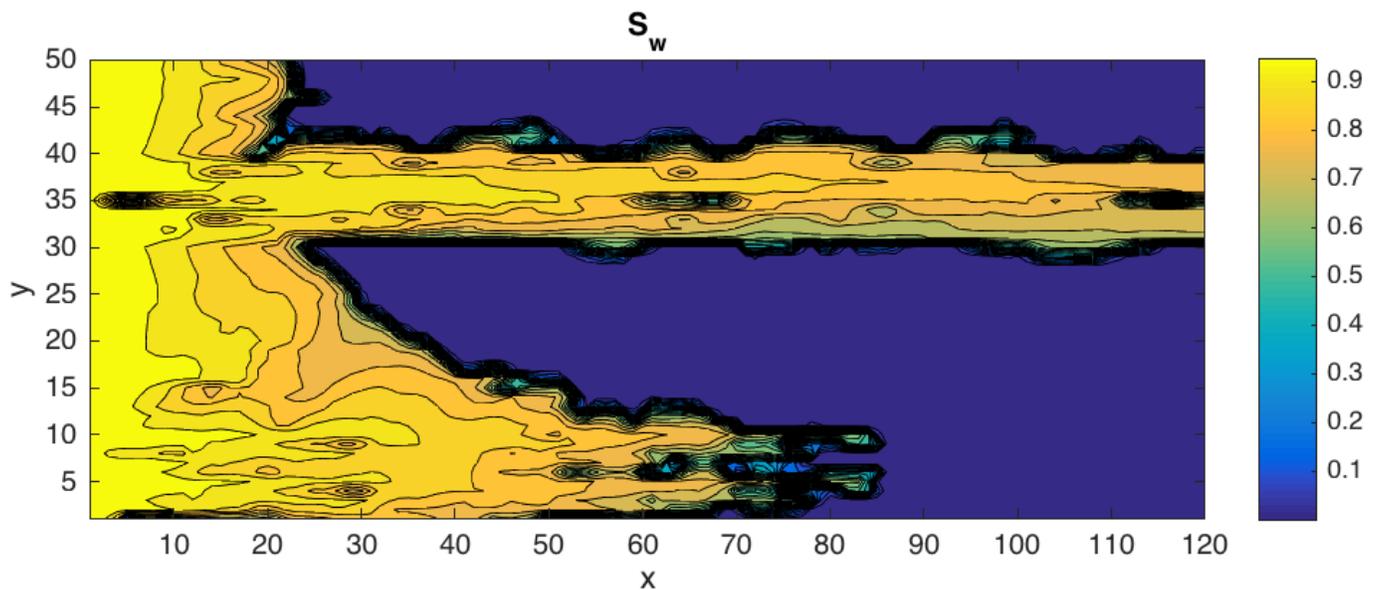


Fig. 7. Distribution of water saturation at 0.5 PV.

Variations of saturation at 0.3 PV, 0.4 PV and 0.5 PV are plotted in Figs. 5, 6 and Fig. 7, respectively. It can be seen from these figures that the distribution for water saturation is discontinuous due to the high heterogeneity of the permeability. One notices the higher water saturation at higher permeability regions.

6. Conclusions

In this paper, we introduce an efficient time-stepping

scheme with adaptive time-step sizes based on the CFL calculation. Hence, we have calculated the CFL_x and CFL_y at each sub-step and checked if the CFL condition is satisfied (i.e. $CFL < 1$). We applied this scheme with IMPES scheme to simulate the problem of two-phase flow in porous media. The capillary pressure is linearized and employed to couple the pressure and the saturation equations. Then, the saturation equation is solved explicitly to update the saturation at each step. The CCFD method was used to discretize the governing equations spatially. In order to show the efficiency of the

proposed scheme, we presented some numerical experiments. The outer pressure time-step size is selected then the saturation subtime-step is calculated and adaptive by the CFL condition. We presented different values of the outer pressure time-step, and distributions of the water saturation is shown in a graph.

Open Access This article is distributed under the terms and conditions of the Creative Commons Attribution (CC BY-NC-ND) license, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

References

- Al-Dhafeeri, A.M., Nasr-El-Din, H.A. Characteristics of high-permeability zones using core analysis, and production logging data. *J. Pet. Sci. Eng.* 2007, 55: 18-36.
- Arbogast, T., Yotov, I., Wheeler, M.F. Mixed finite elements for elliptic problems with tensor coefficients as cell-centered finite differences. *SIAM J. Numer. Anal.* 1997, 34(2): 828-852.
- Belytschko, T., Lu, Y.Y. Convergence and stability analyses of multi-time step algorithm for parabolic systems. *Appl. Mech. Eng.* 1993, 102(2): 179-198.
- Bhalla, S.M., Panday, S., Huyakorn, P.S. Sub-timing in fluid flow and transport simulations. *Adv. Water Resour.* 2003, 26(5): 477-489.
- Chen, Z., Huan, G., Ma, Y. *Computational Methods for Multiphase Flows in Porous Media*. Philadelphia, USA, SIAM Computational Science and Engineering, 2006.
- Coats, K.H. Impes stability: Selection of stable timesteps. Paper SPE 84924 Presented at SPE Reservoir Simulation Symposium, Houston, TX, June, 2001.
- El-Amin, M.F., Kou, J., Salama, A., et al. An iterative implicit scheme for nanoparticles transport with two-phase flow in porous media. *Procedia Comput. Sci.* 2016, 80: 1344-1353.
- El-Amin, M.F., Kou, J., Sun, S. Convergence analysis of the nonlinear iterative method for two-phase flow in porous media associated with nanoparticle injection. *Int. J. Numer. Meth. Heat Fluid Flow* 2017a, 27(10): 2289-2317.
- El-Amin, M.F., Kou, J., Sun, S. A multiscale time-splitting discrete fracture model of nanoparticles transport in fractured porous media. Paper SPE 188001 Presented at SPE Kingdom of Saudi Arabia Technical Symposium and Exhibition, Dammam, Saudi Arabia, 24-27 April, 2017b.
- El-Amin, M.F., Kou, J., Sun, S. Multiscale adapted time-splitting technique for nonisothermal two-phase flow and nanoparticles transport in heterogeneous porous media. Paper SPE 186047 Presented at SPE Reservoir Characterisation and Simulation Conference and Exhibition, Abu Dhabi, UAE, 8-10 May, 2017c.
- El-Amin, M.F., Kou, J., Sun, S. Discrete-fracture-model of multi-scale time-splitting two-phase flow including nanoparticles transport in fractured porous media. *J. Comput. Appl. Math.* 2017d, 333: 327-349.
- Gravouil, A., Combescure, A. Multi-time-step explicit-implicit method for non-linear structural dynamics. *Int. J. Numer. Meth. Eng.* 2000, 50(1): 199-225.
- Hoteit, H., Firoozabadi, A. Numerical modeling of two-phase flow in heterogeneous permeable media with different capillarity pressures. *Adv. Water Resour.* 2008, 31: 56-73.
- Klisiński, M. Inconsistency errors of constant velocity multi-time step integration algorithms. *Comput. Assisted Mech. Eng. Sci.* 2001, 8(1): 121-139.
- Kou, J., Sun, S. A new treatment of capillarity to improve the stability of impes two-phase flow formulation. *Comput. Fluids* 2010, 39(10): 1923-1931.
- Kou, J., Sun, S., Yu, B. Multiscale time-splitting strategy for multiscale multiphysics processes of two-phase flow in fractured media. *J. Appl. Math.* 2011, 4: 1-21.
- Lu, Q. A parallel multi-block/multi-physics approach for multi-phase flow in porous media. Austin, The University of Texas, 2000.
- Park, Y.J., Sudicky, E.A., Panday, S., et al. Application of implicit sub-time stepping to simulate flow and transport in fractured porous media. *Adv. Water Resour.* 2008, 31(7): 995-1003.
- Singh, V., Bhalla, S.M. Complete hydrodynamic border-strip irrigation model. *J. Irrig. Drain. Div.* 1996, 122(4): 189-197.
- Singh, V., Bhalla, S.M. Hydrodynamic modeling of basin irrigation. *J. Irrig. Drain. Eng.* 1997, 123(6): 407-414.
- Smolinski, P., Belytschko, T., Neal, M. Multi-time-step integration using nodal partitioning. *Int. J. Numer. Meth. Eng.* 1988, 26(2): 349-359.
- Smolinski, P., Sleith, S., Belytschko, T. Stability of an explicit multi-time step integration algorithm for linear structural dynamics equations. *Comput. Mech.* 1996, 18(3): 236-243.
- Sun, S., Geiser, J. Multi-scale discontinuous Galerkin and operator-splitting methods for modeling subsurface flow and transport. *Int. J. Multiscale Comput. Eng.* 2008, 6(1): 87-101.
- Telytschko, T., Lu, Y.Y. Convergence and stability analyses of multi-time step algorithm for parabolic systems. *Appl. Mech. Eng.* 1993, 102(2): 179-198.
- Vanderkwaak, J.E. Numerical simulation of flow and chemical transport in integrated surface-subsurface hydrologic systems. Canada, University of Waterloo, 1999.
- Wang, Y., Sun, S., Yu, B. Acceleration of gas flow simulations in dual-continuum porous media based on the mass-conservation POD method. *Energies* 2017, 10(9): 1380.
- Wang, Y., Yu, B., Cao, Z., et al. A comparative study of POD interpolation and POD projection methods for fast and accurate prediction of heat transfer problems. *Int. J. Heat Mass Transf.* 2012, 55(17): 4827-4836.
- Young, L.C., Stephenson, R. A generalized compositional approach for reservoir simulation. *SPE J.* 1983, 23(23): 727-742.