**Editorial**

**Advanced numerical modeling and algorithms for multiphase flow and transport**

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The phenomena of multiphase flow and transport are common in nature and engineering. Modeling and simulation of multiphase flow and transport processes are crucial for a wide range of scientific and industrial applications at various spatial and temporal scales. The past decades have seen remarkable advances in this area, and meanwhile the accurate modeling and efficient, robust simulation of complex multiphase flow and transport still remain challenging. To highlight the recent advances and/or challenges in mathematical and numerical modeling, algorithm, and computation of multiphase flow and transport, we organized a special issue on “advanced numerical modeling and algorithms for multiphase flow and transport” within Journal of Computational Physics.

This special issue presents a total of 17 invited manuscripts contributed from influential worldwide universities, colleges and institutes. These manuscripts cover major topics relevant to the numerical modeling and algorithms for multiphase flow and transport; they not only present the ongoing researches but also show observations of general trends in predictable future. The 17 articles can be classified into five groups and a brief summary of each group is given below.

Group A includes a number of new numerical methods. With increased complexity of the multiphase flow and transport processes, more advanced numerical models, schemes and algorithms are demanded in the direct simulation. In this special issue, Cao et al. [3] developed a coupled volume-of-fluid (VOF) and level set (LS) method based on general curvilinear grids with accurate surface tension calculation. The coupled method combines the advantages of VOF and LS approaches for solving unsteady two-phase flows in irregular domains. Liu et al. [7] presented an efficient numerical algorithm for solving viscosity contrast Cahn–Hilliard–Navier–Stokes two-phase flow system in porous media. The adopted diffuse interface model allows for moving contact line and varying wettability, and the proposed algorithm is validated numerically robust for large-scale 3D simulations. Zhang et al. [15] conducted a comparative study for two interfacial flow modeling approaches: an arbitrary Lagrangian Eulerian finite element method on interface-conforming meshes and a phase field lattice Boltzmann method (LBM) on Cartesian meshes with quadtree adaptive mesh refinement. The phase field LBM is observed to be more dissipative due to the nature of the diffuse interface method used to capture the interfaces. Schneider et al. [9] proposed a hybrid method for free flow/porous-medium flow coupling problems. In this method, a staggered-grid finite volume method (FVM) with good stability is employed to solve the Navier-Stokes equation in the free-flow subdomain and a MPFA FVM with good consistency is used to solve Darcy flow in porous media. Arbogast et al. [2] presented finite volume weighted essentially non-oscillatory (WENO) schemes for nonlinear parabolic problems with degenerate diffusion on non-uniform meshes. The schemes are third order in both space and time in one and two space dimensions using non-uniform meshes of intervals or quadrilaterals. Chen et al. [4] proposed a framework of the mixed generalized multiscale finite element method (GMsFEM) for solving Darcy’s law in heterogeneous media, where pressure is approximated in a multiscale function space that is between fine-grid space and coarse-grid space.
and velocity is approximated directly in the fine-grid space.

Group B focuses the treatment of multicomponent systems. The modeling of multiphase flow taking into account the multicomponent, reaction and mechanics still remains a great challenge. In this special issue, Lu and Wheeler [8] formulated a three-way coupling for both single phase flow and equation-of-state (EOS) compositional flow in a poroelastic medium. The core idea is to determine if the mechanics equation must be solved and whether the fixed-stress iterative coupling is necessary through an error indicator at each time step. Sun [10] established a novel energy-based framework to model multi-component two-phase fluid systems at equilibrium at Darcy’s scale, in which the Peng-Robinson EOS is used to model the bulk properties of each phase. The gravity and capillarity effects are modeled by introducing terms into the total Helmholtz free energy expression. This model is the first effort in the literature that rigorously incorporates capillarity and gravity effects into EOS-based phase equilibrium modeling. Teng and Zhang [12] provided a comprehensive comparison of the equilibrium and kinetic models in the simulation of multiphase, multicomponent, and non-isothermal reactive transport in porous media. Taking the hydrate reaction as example, they found the relative strength of the hydrate reaction and other physical processes controls the magnitude of the differences between these two models.

Group C consists of various approaches for uncertainty quantification (UQ). In nature and engineering, uncertainties are ubiquitous at various spatial and temporal scales. How to quantify the effects of uncertainties on multiphase flow and transport is tricky and less mature. In this special issue, Tarakanov and Elsheikh [11] discussed the polynomial chaos expansion (PCE) that is commonly used for uncertainty quantification (UQ) of quantities of interests obtained from numerical models. They introduced an efficient method for estimating the PCE coefficients combining Elastic Net regularization with a data-driven feature ranking approach. The application to a two-phase subsurface flow and a simulation dataset for CO$_2$ sequestration show the proposed approach resulted in a significant increase in PCE convergence rates. For UQ in modeling coupled stochastic Stokes-Darcy problem with non-stationary porous media, Ambartsouman et al. [1] applied the non-overlapping domain decomposition algorithm to reduce the global problem to a coarse scale mortar interface problem, which is solved by an iterative solver for each stochastic realization. To reduce the computational cost, two algorithms based on deterministic and stochastic multiscale flux basis were introduced. The use of the multiscale flux basis avoids the need for subdomain solves on each iteration and leads to significant savings in computational cost.

Group D concerns applications of machine/deep learning technologies. Machine learning or deep learning has been a powerful tool in multiple research fields. Applying the machine/deep learning to speed up simulations of complex multiphase flow and transport is a vivid research area currently. In this special issue, Wang et al. [14] designed a novel deep neural network model reduction approach for multiscale simulations in porous media. In this approach, they formulated and learned input-output maps constructed with non-local multicontinuum on a coarse grid using multi-layer learning techniques, then they constructed a reduced-order model for the solution approximation using the trained neural network approximation of the input-output map. To relieve the heavy computational burden of phase equilibrium calculations in reservoir compositional simulations, Wang et al. [13] developed an improved artificial neural network model to achieve the prediction of phase stability with high accuracy and reduce the computational costs in order of magnitude.

Group E demonstrates important engineering applications. Multi-applications of multiphase
flow and transport in practical engineering and real-world problems have attracted increased attentions in recent years. In this special issue, Zidane and Firoozabadi [17] presented a higher-order numerical model for the simulation of compositional two-phase flow in a domain with non-planar fractures created in hydraulic fracturing. The proposed model and algorithm were capable of simulating all ranges of fracture permeability accurately as opposed to other approaches where low permeability fractures affect the accuracy. Zhong et al. [16] performed numerical simulations of polymer flooding process in porous media on distributed-memory parallel computers. Results show that their computed results match those of the commercial simulator and their simulator possesses excellent speedup demonstrated by large-scale applications with up to 27 million grid blocks using up to 2048 CPU cores. Solovsk and Mikyska [5] studied the dimensional effects of inter-phase mass transfer on attenuation of structurally trapped gaseous carbon dioxide in shallow aquifers. They pointed out the distinctions in CO₂ mass transfer processes between the quasi-1D and 2D cases using a two-phase compositional flow model in heterogeneous porous media. Kumar et al. [6] developed effective upscaled models for replacing a fracture by an interface for Richards’ equation describing flow in an unsaturated porous medium containing a fracture.

We are glad to share above articles in our special issue with relevant communities of interest. Although this special issue cannot cover all the topics in this area, we believe it will provide a valuable volume to readers on the significant advances in the numerical modeling and algorithms for multiphase flow and transport. We sincerely hope the numerical models, algorithms, methods, and all achievements presented in these papers will help to improve the fundamental understanding of the complex multiphase flow and transport processes and solve related challenging scientific and engineering problems. Furthermore, we sincerely hope this special issue can provide a platform for bringing together investigators in this field to exchange the latest research ideas, and to promote further collaborations.

We would like to sincerely acknowledge all the authors for their inspiring contributions to this special issue. We also would like to thank the anonymous reviewers for their diligent, helpful and constructive comments that greatly contributed to improving the overall quality of the manuscripts. Finally, our thanks are extended to Journal of Computational Physics for providing a wonderful opportunity to organize this special issue. The managing guest editor Shuyu Sun and the guest editor Bo Yu also express their sincere gratitude to the great support from the National Natural Science Foundation of China (51874262, 51936001, and 51904031) and the Research Funding from King Abdullah University of Science and Technology (KAUST) through the grants BAS/1/1351-01, URF/1/3769-01, and REP/1/2879-01.

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