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Pore-scale fluid flow simulation coupling lattice Boltzmann method and pore network model

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Abstract:
The lattice Boltzmann method and pore network model are two types of the most popular pore-scale fluid flow simulation methods. As a direct numerical simulation method, lattice Boltzmann method simulates fluid flow directly in the realistic porous structures, characterized by high computational accuracy but low efficiency. On the contrary, pore network model simulates fluid flow in simplified regular pore networks of the real porous media, which is more computationally efficient, but fails to capture the detailed pore structures and flow processes. In past few years, significant efforts have been devoted to couple lattice Boltzmann method and pore network model to simulate fluid flow in porous media, aiming to combine the accuracy of lattice Boltzmann method and efficiency of pore network model. In this mini-review, the recent advances in pore-scale fluid flow simulation methods coupling lattice Boltzmann method and pore network model are summarized, in terms of single-phase flow, quasi-static two-phase drainage flow and dynamic two-phase flow in porous media, demonstrating that coupling the lattice Boltzmann method and pore network model offers a promising and effective approach for addressing the up-scaling problem of flow in porous media.

1. Introduction

Fluid flow in porous media is a common phenomenon in many science and engineering processes (Cai et al., 2021; Diao et al., 2021; Liu et al., 2022), such as oil and gas field development, geological CO_2 storage, water management in fuel cells, etc. In recent years, with the fast development of imaging techniques and computing power, pore-scale experiments (Blunt et al., 2013) and numerical modeling (Zhao et al., 2019) are playing an increasingly important role in helping to understand the microscopic flow mechanisms in porous media. Compared with pore-scale experiments, pore-scale numerical simulation is relatively low-cost, flexible in controlling variables and can provide detailed flow, pressure and phase distributions inside the complex pore space, making it more suitable for mechanism analysis.

There are two types of pore-scale numerical methods, the direct numerical simulation (DNS) methods and pore network model (PNM). The DNS methods simulate fluid flow directly in the realistic porous structures, which can be obtained by imaging techniques or reconstruction method (Blunt et al., 2013). As one kind of DNS method, lattice Boltzmann method (LBM) has become a very popular pore-scale numerical method for flow simulation in porous media due to its kinetic nature, programming simplicity, intrinsic parallelism and great advantage in treating the complex solid boundaries (Chen et al., 2022). However, it involves the collision-migration evolution of discrete fluid particles within lattice cells, making it computationally demanding. This characteristic poses

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challenges when dealing with the flow problem in large-scale porous media domains and becomes more pronounced in the presence of multiphase flow. Consequently, current LBM research often confines computations to 2-dimensional spaces or 3-dimensional models with a limited number of grids per side to facilitate systematic parametric analysis (Huang et al., 2015). This is a common issue for all DNS methods. On the contrary, in the PNM, the complex pore structures are firstly simplified into regular pore bodies and throat bonds based on some criteria, resulting in a simplified pore network of the real porous medium. With such simplification, the Darcy-type equation is used in PNM to describe the fluid flow process, instead of the more complicated Navier-Stokes equation, making the PNM much more computational efficient. Therefore, PNM can be used in flow simulations in large porous media domains with advanced parallel algorithms (Gong et al., 2020). However, the PNM sacrifices computational accuracy due to simplifications in pore structure and fluid flow (Joekar-Niasar et al., 2012).

By combining the detailed and accurate representation of pore-scale physics provided by LBM with the computational efficiency and retention of realistic pore space topology offered by PNM, coupling the LBM and PNM offers a promising and effective approach for addressing the up-scaling problem in porous media (Mukherjee et al., 2011). In this mini-review, the recent advances in pore-scale fluid flow simulation coupling lattice Boltzmann method and pore network model are summarized.

2. Single-phase flow in porous media

Single-phase flow in porous media is a process in which only one fluid completely occupies the pore space. Since there are no unstable two-fluid interface interactions in the flow process, the single-phase flow characteristics depend primarily on the complexity of the porous structure. Accordingly, accurate description of the real pore structure is important, especially for the narrow throats, which accounts for most of the flow resistance. In the conventional PNM, the pore bodies and throat bonds are simplified into regular shapes, making it less accurate in throat conductance characterization and permeability calculation (Zhao et al., 2020a). Different improvements were proposed to incorporate more shape information in the single-phase PNM. Prodanović et al. (Prodanović et al., 2007) and Sholokhova et al. (Sholokhova et al., 2009) proposed to use the real throat instead of a simplified column in pore network extraction. The lattice Boltzmann computations were used to calculate the conductance of each individual throats, based on which a correlation between conductance and throat cross-sectional area was fitted. Similarly, Van Marcke et al. (2010) decomposed the pore space into sub-pore regions based on watershed method and the throat bonds characterized by pore-throat-pore elements were extracted. The computational fluid dynamics (CFD) method was used to calculate the local conductance of each pore-throat-pore element and then PNM was used to obtain the permeability of the whole porous medium. In above studies, the real throat geometry without shape simplification was used in the PNM simulations, as shown in Fig. 1(b), thus providing more accurate permeability values.

As the throat information is most important for single-phase flow in porous media, another improvement is to use the real throat cross section to replace the regular one in the conventional PNM (Miao et al., 2017; Rabbani et al., 2019), as schematically shown in Fig. 1(c). Then the conductance of the real throat cross section can be calculated by direct numerical simulation methods such as CFD method and LBM (Miao et al., 2017; Rabbani et al., 2019). To further improve the computational efficiency, the neural network model was further used to relate the single-phase conductance with the shape information of real throat cross section. It was found the mean distance to solid surface showed dominant role in determining the throat conductance. As more realistic throat geometry was considered, the improved PNM usually predicts more accurate single-phase permeability.

Recently, Zhao et al. (2020a) proposed another improved PNM for single-phase flow, which uses a serial of sub-throat bonds with real cross sections to further capture the cross section variations between two pore bodies, as shown in Fig. 1(d). The conductance of each sub-throat bond was also calculated by LBM simulations. In addition, the accuracy of the above mentioned three different improved PNMs, as shown in Figs. 1(b)-1(d), were verified with the whole domain LBM simulations in three sandstone digital rocks, in terms of both permeability and detailed pressure distributions. The results showed that, with more shape information considered, the accuracy of PNM in predicting permeability increases, at the expense of computational efficiency. The PNM with real throat geometry can replace the whole domain LBM simulation with much lower computational cost. While the PNM with serial sub-throat bonds is a better choice for single-phase flow simulation which has the best balance between accuracy and computational cost.

3. Quasi-static two-phase flow in porous media

PNMs have been widely used to simulate two-phase flow at low flow velocities within porous media, employing quasi-static flow models (Bultreys et al., 2015). This approach assumes that the flow behavior is predominantly governed by capillary forces, while viscous forces are negligible. During the quasi-static drainage process, where the non-wetting phase preferentially invades the large pores and throats, the flow characteristics are predominantly controlled by the throat cross-section, thus allowing the invasion-percolation theory to accurately capture the invading sequence. Nevertheless, due to the simplification of throat shapes in conventional PNM, discrepancies may arise when dealing with real pore structures. In addition, for layered two-phase flow in a single throat, the flow of one fluid will cause the movement of the other fluid due to the viscous drag force at the interface, known as viscous coupling effect. The viscous coupling effect is generally neglected in the conventional PNM, making PNM less reliable when calculating the relative permeability curve, especially for the non-wetting fluid.

Significant efforts have been devoted to improve the accu-

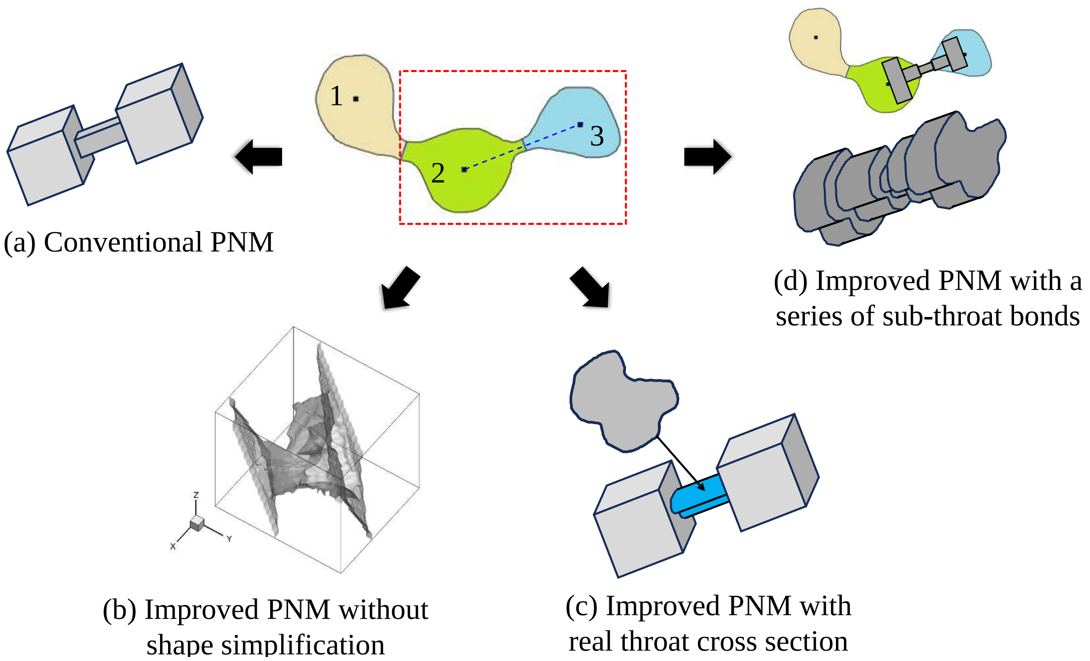

Fig. 1. Schematics of different pore network models for single-phase flow in porous media.

racy of conventional PNM with the help of direct numerical method. To incorporate the viscous coupling effect, the direct numerical methods (CFD or LBM) were used to simulate layered two-phase or three-phase flow across regular throat bonds to calculate the corresponding conductance (Dehghanpour et al., 2011; Xie et al., 2017; Shams et al., 2018; Jiang et al., 2021). Different conductance calculating models were proposed considering the viscous coupling effect, which could be further incorporated into the quasi-static PNM. The simulation results with the modified conductance considering viscous coupling effect showed better agreement with experimental data, demonstrating the significance of viscous coupling effect on two-phase flow (Xie et al., 2017).

The direct numerical simulation methods can be also used to determine the exact interfacial configurations in the pore space, thus providing more accurate descriptions of the pore-level flow process. Giudici et al. (2023) used the generalized network model to simulate quasi-static two-phase flow in porous media, where the corners were used to discretize the pore space to better capture the pore geometry. The direct numerical simulations were used to validate and calibrate the threshold capillary pressures of the invading fluid when passing through these more realistic pore geometries under different wetting conditions. To more accurately characterize the throat geometry, Suh et al. (2017) proposed to use the real throat cross section instead of the regular one to determine the threshold capillary pressure. Both the LBM simulations and Mayer-Stowe-Princen theory were used to calculate the threshold capillary pressure values of these irregular throat bonds. The water retention curves obtained by the improved PNM agreed well with experimental data. However, the relative permeability curve were not obtained. Zhao et al. (2020b) also used the real throat cross section in the PNM simulation to replace the simplified regular one, as shown in Fig. 2. The two-phase flow parameters across these real throat cross sections were determined by the color-gradient LBM simulations, including the threshold capillary pressure, the capillary pressure - saturation relationship, the single-phase conductance and relative conductance - saturation relationship. In addition, to further improve the computational efficiency, the artificial neural network (ANN) model was adopted to link the two-phase flow parameters with the throat shape information based on a large amount of LBM simulations in different cross sections. Both the conventional and improved PNMs were used to simulate quasi-static drainage flow in a Berea sandstone and the obtained relative permeability curves were compared with the experimental results. As expected, the improved PNM better predicted the relative permeability curve, especially for the non-wetting phase. Montellá et al. (2020) developed a hybrid method coupling LBM and PNM for quasi-static drainage in granular porous media, where the quasi-static PNM was used to determine the invading sequence, while the LBM was used to calculate the capillary pressure - saturation relationship in a single pore element without shape simplification. This hybrid method accurately reproduced the fluid movement during drainage process compared with full-domain LBM simulation.

4. Dynamic two-phase flow in porous media

With the increase of two-phase flow velocity, the viscous force becomes non-negligible and the quasi-static PNM becomes invalid. At such conditions, the dynamic pore network model (Joekar-Niasar et al., 2012) or direct numerical simulation methods (Zhao et al., 2019) should be used to describe the two-phase dynamics. In recent years, different DNS-PNM coupling schemes were developed to simulate dynamic two-

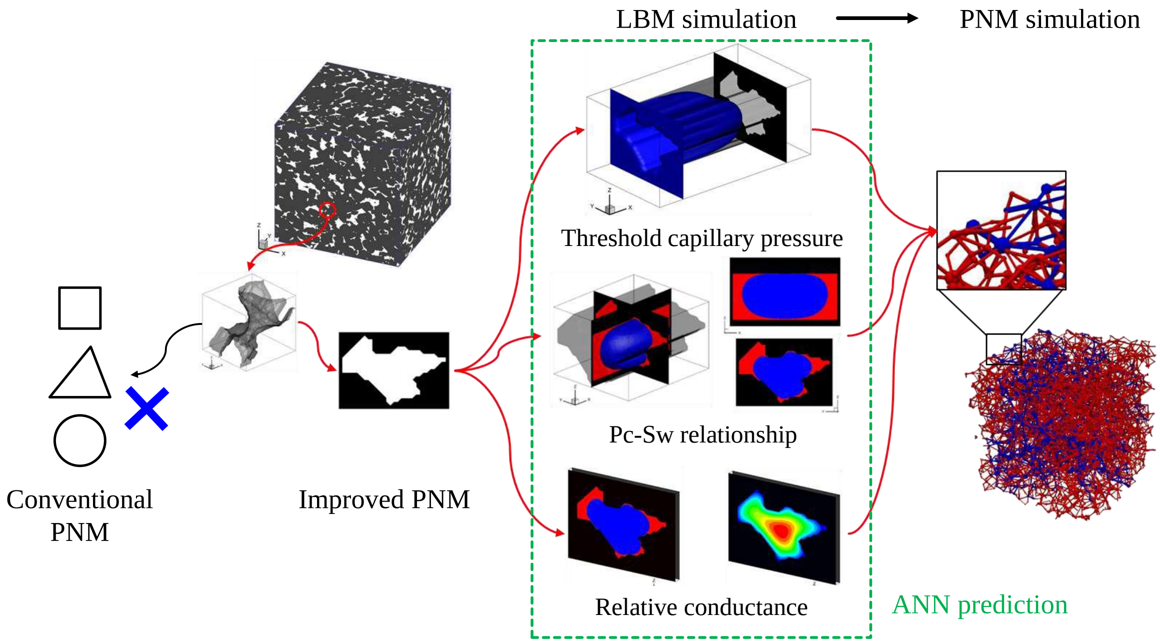

Fig. 2. Improved pore network model for quasi-static drainage simulation coupling lattice Boltzmann method and pore network model.

phase flow in porous media, aiming to combine the accuracy of DNS and efficiency of PNM.

Mehmani et al. (Mehmani et al., 2019) developed a pore-level multiscale method (PLMM) for two-phase flow in porous media, where the basis functions were constructed for single-phase flow, while the correction functions were designed for two-phase interactions. By treating the two-phase dynamics as local perturbations to single-phase flow, this multiscale method localized the computations to the displacement front. With similar idea, Zhao et al. (2021) proposed a hybrid lattice Boltzmann - pore network model to simulate liquid drying from porous media, as illustrated in Fig. 3. Fig. 3(a) shows the liquid (red) and vapor (blue) distributions in a porous medium at a certain time. Based on watershed method, the pore space can be decomposed into sub-pore regions. Then the phase distribution can be mapped to the sub-pore region distribution, resulting in different types of pore elements, as shown in Fig. 1(b), including the two-phase pores shown in yellow where the two-phase interfaces exist; the single-liquid and single-vapor phase pores shown in red and blue, respectively; and the green buffer pores which connect the single-phase pores and two-phase pores. In the simulation, the pseudo-potential LBM is used in the two-phase and buffer pores to simulate liquid drying and track the movement of the interfaces, while the PNM simulations are conducted in the buffer and single-phase pores to simulate liquid and vapor flow. The LBM and PNM are coupled in the buffer pores through a novel boundary condition, as illustrated in Fig. 3(c). The accuracy of the hybrid model is verified with the whole-domain LBM simulation of liquid drying from different porous media. The hybrid method always produces almost identical results compared with the whole-domain LBM simulations with much less computational cost, demonstrating its superiority. In addition, the speedup of the hybrid method becomes more significant for a larger computational domain.

The hybrid DNS-PNM algorithm was more often designed for the two-phase interactions with a free surface. K. Weishaupt et al. (2019, 2021) developed a DNS-PNM coupling method to simulate liquid evaporation from the porous media to a free-flow domain, where the dynamic two-phase two-component PNM was used to simulate liquid transport and evaporation in the porous domain, while the DNS method was used in the free-flow domain. A monolithic coupling scheme was proposed to ensure the conservation of mass, momentum and energy across the coupling interface. Suo et al. (2020) studied the droplet spreading on porous surface with a LBM-PNM framework. Similarly, a two-phase LBM model was used in the free surface domain to capture the droplet dynamics above the porous surface, while the dynamic two-phase PNM was employed in the porous matrix domain. An effective transport mechanism was implemented to guarantee mass conservation and pressure continuity across the interface. These coupling methods successfully combine the accuracy of DNS and efficiency of PNM.

5. Conclusions

In this mini-review, the recent advances in pore-scale fluid flow simulation methods coupling lattice Boltzmann method and pore network model are summarized, in terms of single-phase flow, quasi-static two-phase drainage flow and dynamic two-phase flow in porous media. For single-phase flow in porous media, three types of improved pore network models were developed. With more shape information considered, the accuracy of PNM in predicting permeability increases, at the expense of computational efficiency. For quasi-static two-phase drainage flow, significant efforts have been devoted in

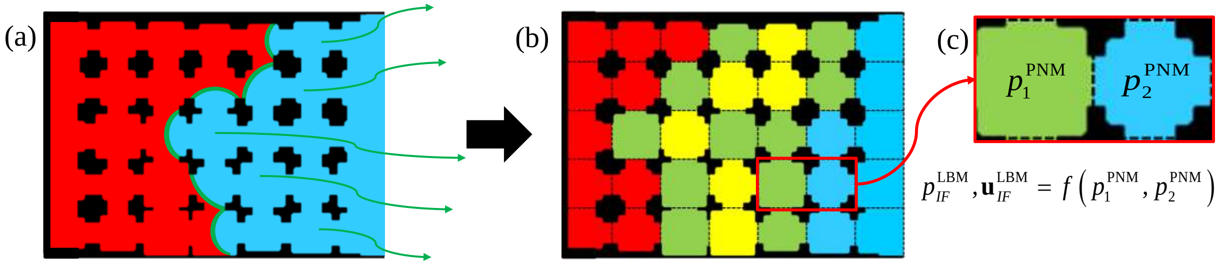

Fig. 3. Hybrid lattice Boltzmann - pore network model for drying simulation in porous media. (a) Phase distribution, (b) pore-type distribution and (c) boundary condition. p is pressure, $\mathbf{u}$ is velocity, the subscript "IF" means interface.

incorporating the viscous coupling effect and improving the accuracy of threshold capillary pressure of throat bonds or capillary pressure - saturation relationship of pore bodies, with the help of direct numerical simulation methods. For dynamic two-phase flow in porous media, the direct numerical simulation method and pore network model were used to simulate fluid flow in different computational domains, and different coupling schemes were developed to exchange information at the interface between them. In summary, the LBM-PNM coupling methods have been proved to be a promising and effective approach for addressing the up-scaling problem of flow in porous media.

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Conflict of interest

The authors declare no competing interest.

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