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Lattice Boltzmann Modeling of Multicomponent Fluid Flow in Multiscale Porous Media

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Abstract. Since its development, the lattice Boltzmann method (LBM) has proven to be an excellent tool for simulating multiphase/multicomponent fluid flows through porous media. Rooted in the kinetic theory of particles, the method effectively models the interactions at fluid interfaces between different phases. However, in the LBM literature, the multiphase/multicomponent multiscale approaches usually keep the fluid segregation term within the porous-continuous media (PCM), thereby clearly identifying the immiscible fluid interface. This aspect eliminates the relative permeability resistance and the capillary pressure effects during fluid-fluid displacement, making it solely dependent on absolute permeability. Therefore, the present work proposes a multiscale multicomponent modeling by incorporating the non-linearity of relative permeability resulting from fluid–fluid interactions within the PCM region. To achieve this, the study combines pore-scale immiscible flow, represented by the Navier-Stokes equations, with the Buckley–Leverett equation to describe the non-linear mass balance of the two components. Additionally, the generalized porous continuous Navier-Stokes equation proposed by [1] is employed to account for the momentum balance. By integrating these equations, the present work provides a comprehensive framework for modeling the PCM region, effectively capturing both mass and momentum dynamics influenced by non-linear relative permeability (described by Corey [2] correlation) and capillary pressure effects (described by Van Genuchten [3] correlation).

Keywords: Lattice Boltzmann Method, Multicomponent flow, non-unitary mass-ratio

1 Introduction

The lattice Boltzmann approaches to describe multiphase/multicomponent multiscale [4–8] must retain the fluid segregation term within the porous continuous media(PCM) region, thereby clearly identifying the immiscible fluid interface. This aspect eliminates the relative permeability resistance during fluid displacement, making it solely dependent on absolute permeability.

Therefore, the present work aims to extend multiscale multiphase/multicomponent modeling by incorporating the non-linearity of relative permeability resulting from fluid–fluid interactions within the PCM region. To achieve this, the study combines pore-scale immiscible flow, represented by the Navier-Stokes equations, with the Buckley–Leverett equation to describe the non-linear mass balance of the two components. Additionally, the generalized porous continuous Navier-Stokes equation proposed by Nithiarasu et al. [1] is employed to account for the momentum balance. By integrating these equations, the present work provides a comprehensive framework for modeling the PCM region, effectively capturing both mass and momentum dynamics influenced by non-linear relative permeability.

2 Multiscale Binary Mixture Modeling

A multiscale binary mixture model couples mass and momentum balance equations to describe transport phenomena within both the pore-scale and PCM domains, aiming to represent immiscible fluid–fluid displacement. The system is characterized by a binary mixture of two Newtonian fluids, a wetting (w) and a non-wetting (nw), both maintained at a constant temperature.

2.1 Pore-Scale Domain

In describing pore-scale transport phenomena, the mass balance equation is expressed as

$$\partial_t \rho^{(k)} + \partial_\alpha(\rho^{(k)} u_\alpha) + \partial_\alpha(m_\alpha^{(k)}) = 0, \tag{1}$$

where $\rho^{(k)}$ is the fluid density, u_α is the mixture velocity vector, m_α is the mass diffusive vector, and the superscript k indicate the fluid, w or nw. The momentum balance of the mixture can be described by

$$\partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) = -\partial_\beta\left(P_s\delta_{\alpha\beta} + S_{\alpha\beta}\right) + \rho\nu\partial_\beta\left(\partial_\alpha u_\beta + \partial_\beta u_\alpha - 2\partial_\alpha u_\alpha \delta_{\alpha\beta}/3\right) \tag{2}$$

where $P_s = p - \left(\partial_\alpha(\partial_\alpha\rho^2) - \partial_\alpha\rho\partial_\alpha\rho\right)\kappa/2$ is the scalar pressure, p is the fluid thermodynamic pressure, κ is the molecular interaction potential, which is directly related to the interfacial tension between the fluids. The term $S_{\alpha\beta} = \kappa\partial_\alpha(\rho)\partial_\beta(\rho)$ is the Korteweg stress tensor.

2.2 PCM Domain

In the PCM domain, the Buckley–Leverett equation is used to model mass balance, while the generalized Navier–Stokes equation governs momentum balance. The Buckley–Leverett equation, originally proposed by Buckley and Leverett [9], is a nonlinear partial differential equation derived from the mass balance of a binary mixture, employing the concept of fractional flow. In its extended formulation, the Buckley–Leverett equation is given by

$$\partial_t s^{(w)} + \partial_\alpha B_\alpha^{(w)} + \partial_\alpha\left(\lambda^{(w)}\left(C_\alpha^{(w)} - \partial_\alpha\left(\lambda^{(w)}\epsilon^{(w)}\partial_t s^{(w)}\right)\right)\right) = 0, \tag{3}$$

$$\partial_t s^{(nw)} + \partial_\alpha B_\alpha^{(nw)} - \partial_\alpha\left(\lambda^{(nw)}\left(C_\alpha^{(nw)} - \partial_\alpha\left(\lambda^{(nw)}\epsilon^{(nw)}\partial_t s^{(nw)}\right)\right)\right) = 0, \tag{4}$$

where $s^{(k)}$ is the fluid saturation, $B_\alpha^{(k)}$ convective fractional flux vector, $\lambda^{(k)}$ is diffusive constant, $C_\alpha^{(k)}$ diffusive capillary vector, and $\epsilon^{(w)}$ is the dynamic pressure constant. By definition, the terms $B_\alpha^{(k)}$, $\lambda^{(k)}$, $C_\alpha^{(k)}$, and $\epsilon^{(w)}$ are described as:

$$\begin{gathered} B_\alpha^{(k)} = \left(\frac{\langle u_\alpha^p\rangle}{\varphi} + \frac{\langle \bar{u}_\alpha^{(k)}\rangle}{\varphi}\widehat{K}^{(\bar{k})}\right)F^{(k)}, \qquad \langle \bar{u}_\alpha^{(k)}\rangle = \frac{K}{\mu^{(\bar{k})}}g_\alpha^e\left(\rho^{(k)} - \rho^{(\bar{k})}\right), \qquad F^{(k)} = \frac{\widehat{K}^{(k)}\mu^{(\bar{k})}}{\left(\widehat{K}^{(\bar{k})}\mu^{(k)} + \widehat{K}^{(k)}\mu^{(\bar{k})}\right)}, \\ \lambda^{(k)} = \frac{\sigma K}{\varphi\mu^{(\bar{k})}}\sqrt{\frac{\varphi}{K}}, \qquad C_\alpha^{(k)} = F^{(k)}\widehat{K}^{(\bar{k})}\partial_\alpha\widehat{p}_c, \qquad \epsilon^{(k)} = -\frac{\zeta\varphi F^{(k)}}{\lambda^{(k)}} \end{gathered} \tag{5}$$

where φ is the porosity, $\langle u_\alpha^p\rangle = \langle u_\alpha^{(w)}\rangle + \langle u_\alpha^{(nw)}\rangle$ is the mixture average velocity vector, $\langle \bar{u}_\alpha^{(k)}\rangle$ is the average buoyancy vector, $F^{(k)}$ is the fractional flux term, σ is the interfacial tension, $\mu^{(k)}$ is the dynamic viscosity, K is absolute permeability, g_α^e is an external acceleration vector, and the superscript $\bar{k}$ denotes the fluid different from k. The term $\widehat{p}_c(s_k)$ represents the dimensionless capillary pressure, typically specified through correlations (e.g., Van Genuchten 3 correlation). The dimensionless term of relative permeability $\widehat{K}^{(k)}$ is likewise given by correlations dependent on saturation (e.g., Corey 2 correlation). The parameter ζ is the damping or non-equilibrium coefficient, which controls the dynamic capillary effect and can also vary with fluid saturation. The present work follow the definition of average and intrinsic velocities defined by Whitaker [10]:

$$\langle u_\alpha^{(k)}\rangle = \frac{1}{V}\int_{V^{(k)}} u_\alpha^{(k)} dV = \varphi\frac{1}{V^{(k)}}\int_{V^{(k)}} u_\alpha^{(k)} dV = \varphi\langle u\rangle_\alpha^{(k)} \tag{6}$$

where $\langle u\rangle_\alpha^{(k)}$ is intrinsic average velocity. Summing over all fluids in PCM region, the relation between the average and intrinsic average is given by $\langle u_\alpha^p\rangle = \langle u_\alpha^{(w)}\rangle + \langle u_\alpha^{(nw)}\rangle = \varphi(\langle u\rangle_\alpha^{(w)} + \langle u\rangle_\alpha^{(nw)}) = \varphi\langle u\rangle_\alpha^p$.

The momentum balance in the PCM domain is described by the generalized Navier–Stokes equation proposed by Vafai and Tien [11], which governs the momentum evolution of the mixture. However, in the present we employ an adapted form of the generalized Navier–Stokes equation proposed Nithiarasu et al. [1] in terms of average velocity:

$$\partial_t(\rho\langle u_\alpha^p\rangle) + \partial_\beta\left(\rho\langle u_\alpha^p\rangle\langle u_\beta^p\rangle/\varphi\right) = -\partial_\beta\left(\varphi\langle p\rangle^p\right) + \rho\nu_e\partial_\beta\left(\partial_\alpha\langle u_\beta^p\rangle + \partial_\beta\langle u_\alpha^p\rangle\right) - \frac{\varphi\mu}{K}\langle u_\alpha^p\rangle - \frac{\rho\varphi F_e}{\sqrt{K}}|\langle u_\alpha^p\rangle|\langle u_\alpha^p\rangle \tag{7}$$

where ν_e effective viscosity, F_e is geometric factor term from inertial effects in porous media. When $\varphi = 1$, $\nu_e = \nu$, and $K \to \infty$, the generalized Navier–Stokes equation reduces to the usual Navier–Stokes equation.

3 Numerical Results: 1D fluid-fluid displacement

To validate the description of the Buckley-Leveret mass transport inside of the PCM domain, a 1D benchmark is employed to compare the developed saturation profile with analytical and numerical solutions available. The 1D problem geometry is characterized by a inlet and outlet pore-scale domain with L_{ps} length and in the middle a PCM domain of length L_{pcm}, as illustrated in the Figure 1. Considering $\langle u^p_\alpha \rangle = 1$ m/s constant over all domain, porosity $\varphi = 0.1$, dynamic viscosity ratio $M_\mu = 1$, and lengths $L_{ps} = 10$ m and $L_{pcm} = 20$ m. Water is injected at the inlet $(x = 0)$ under a Dirichlet boundary condition $s_w(x = 0) = 1$. At the outlet $(x = L)$, a Neumann boundary condition specifying a zero gradient in water saturation is applied.

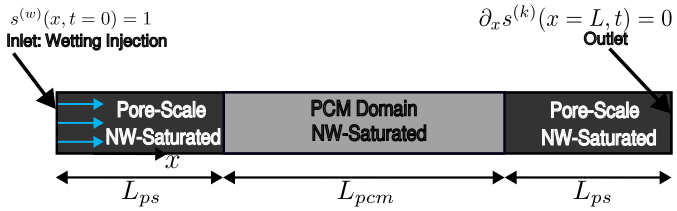


Figure 1. Geometry of 1D fluid-displacement case across consecutive pore-scale and PCM domains.

As a first scenario, we consider a pure convective formulation where gravitational effects and capillary pressure are neglected,

$$\partial_t(s^{(w)}) + \partial_\alpha \left(\frac{\langle u^p_\alpha \rangle}{\varphi} F^{(w)} \right) = 0 \qquad \text{with} \qquad F^{(w)} = \frac{(s^{(w)})^2}{(s^{(w)})^2 + M_\mu (1 - s^{(w)})^2}, \tag{8}$$

where $\widehat{K}^{(w)} = (s^{(w)})^2$, $\widehat{K}^{(nw)} = (s^{(nw)})^2$, i.e., $s_{wi} = s_{nwr} = 0$ and $n_w = n_{nw} = 2$. The non-linear convective problem given by the Eq. (8) has an analytical solution dependent of the initial condition (Riemann problem). In the present case, the solution for the specific initial condition is given by

$$s^{(w)}(x, t) = \begin{cases} tF^{'(w)} & \text{for} \quad x \leq \varsigma t \\ 0 & \text{for} \quad x > \varsigma t \end{cases} \tag{9}$$

where $\varsigma = F^{'(w)}(\tilde{s}^{(w)}) = F^{(w)}(\tilde{s}^{(w)})/\tilde{s}^{(w)}$ is the shock wave speed, $F^{'(w)} = dF^{(w)}/ds$, and $\tilde{s}^{(w)} = \sqrt{M_\mu/(M_\mu + 1)}$ is the sharp front saturation.

Considering $L_{ps} = 10$ m, $L_{pcm} = 20$ m, $\Delta x = 0.008$ m, and $\Delta s = 0.002$ s, these parameters yields $L_{ps} = 1250$ lu, $L_{pcm} = 2500$ lu, and $\langle u^p_\alpha \rangle^* = 0.025$. The saturation profiles for water and oil and water field saturation are plot at the time $t^* = 8000$, 20000 , 30000 and 35000 in the Figures 2 a), b) c), and d), respectively.

At the inlet scale transition from the pore-scale to the PCM region, both fluids coexist at the same site, as represented by the Buckley–Leverett equation. Comparing the saturation profile at $t^* = 20000$ to the analytical solution, we observe good agreement between the numerical and analytical results.

Notice that once the shock wave passes through the outlet porous transition interface, both fluid saturations are transferred from the PCM to the pore-scale region at the same lattice node. At the pore scale, the segregation forces begins to act again, segregating the fluid components, as illustrated in Figure 2 c) and d). Due to the one-dimensional nature of the problem, the fluid components separate into layers of water and oil.

4 Conclusions

The present lattice Boltzmann formulation for multiscale multiphase/multicomponent systems is capable of describing fluid–fluid interactions across different porous media representations, while satisfying mass and momentum balance at the interfaces between scales. Additionally, for the one-dimensional fluid–fluid displacement case, the results show good agreement with the analytical solution within the PCM region.

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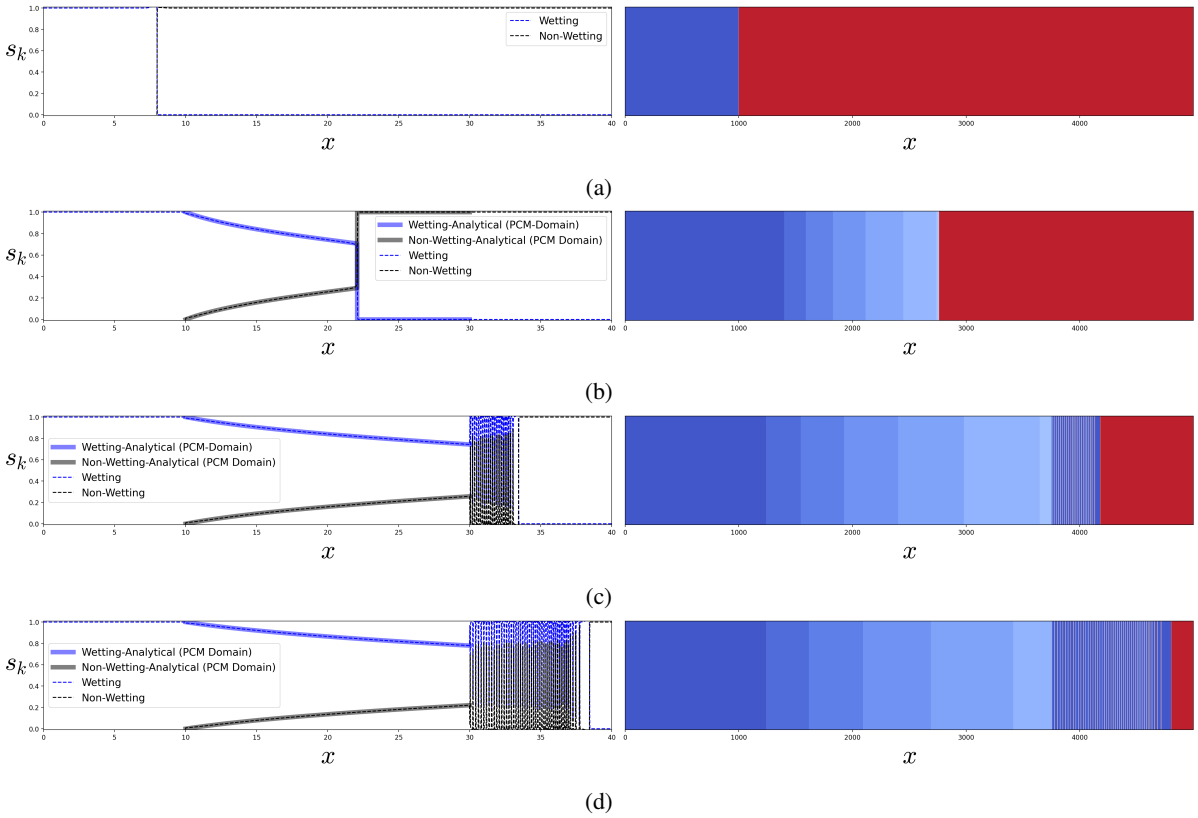


Figure 2. Numerical solutions of wetting and non-wetting saturation profile for different times steps: (a) $t^* = 8000$ ts, (b) $t^* = 20000$ ts, (c) $t^* = 30000$ ts, and (d) $t^* = 35000$ ts. The thick blue and black lines inside of PCM domain range in the curves of saturation profile describe the predicted analytical solution taking as reference the time when the wetting fluid enters the PCM domain.

References

[1] P. Nithiarasu, K. Seetharamu, and T. Sundararajan. Natural convective heat transfer in a fluid saturated variable porosity medium. *International Journal of Heat and Mass Transfer*, vol. 40, n. 16, pp. 3955–3967, 1997.

[2] A. T. Corey. The interrelation between gas and oil relative permeabilities. *Producers monthly*, vol. 1, pp. 38–41, 1954.

[3] M. T. Van Genuchten. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. *Soil science society of America journal*, vol. 44, n. 5, pp. 892–898, 1980.

[4] M. A. Spaid and F. R. Phelan Jr. Modeling void formation dynamics in fibrous porous media with the lattice boltzmann method. *Composites Part A: Applied Science and Manufacturing*, vol. 29, n. 7, pp. 749–755, 1998.

[5] P. McDonald and M. Turner. Combining effective media and multi-phase methods of lattice boltzmann modelling for the characterisation of liquid-vapour dynamics in multi-length scale heterogeneous structural materials. *Modelling and Simulation in Materials Science and Engineering*, vol. 24, n. 1, pp. 015010, 2015.

[6] G. G. Pereira. Grayscale lattice boltzmann model for multiphase heterogeneous flow through porous media. *Physical Review E*, vol. 93, n. 6, pp. 063301, 2016.

[7] Y. Ning, C. Wei, and G. Qin. A unified grayscale lattice boltzmann model for multiphase fluid flow in vuggy carbonates. *Advances in Water Resources*, vol. 124, pp. 68–83, 2019.

[8] Y. Liu, J. Feng, J. Min, and X. Zhang. Homogenized color-gradient lattice boltzmann model for immiscible two-phase flow in multiscale porous media. *Journal of Applied Physics*, vol. 135, n. 18, 2024.

[9] S. E. Buckley and M. Leverett. Mechanism of fluid displacement in sands. *Transactions of the AIME*, vol. 146, n. 01, pp. 107–116, 1942.

[10] S. Whitaker. Flow in porous media i: A theoretical derivation of darcy's law. *Transport in porous media*, vol. 1, pp. 3–25, 1986.

[11] K. Vafai and C. L. Tien. Boundary and inertia effects on flow and heat transfer in porous media. *International Journal of Heat and Mass Transfer*, vol. 24, n. 2, pp. 195–203, 1981.