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Lattice Boltzmann Method for Diffusion-Reaction-Transport Processes in Heterogeneous Porous Media *

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Based on the lattice Boltzmann method and general theory of fluids flowing in porous media, a numerical model is presented for the diffusion-reaction-transport (DRT) processes in porous media. As a test, we simulate a DRT process in a two-dimensional horizontal heterogeneous porous medium. The influence of gravitation in this case can be neglected, and the DRT process can be described by a strongly heterogeneous diagnostic test strip or a thin confined piece of soil with stochastically distributing property in horizontal directions. The results obtained for the relations between reduced fluid saturation S, concentration c_1, and concentration c_2 are shown by using the visualization computing technique. The computational efficiency and stability of the model are satisfactory.

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In the past several decades, the diffusion-reaction-transport (DRT) process in porous media has attracted considerable attention due to its important applications for geothermal energy systems, new diagnostic test strips, secondary and tertiary oil recovery, prevention of subsoil water pollution, and other related topics. To the best of our knowledge, the DRT process in porous media is treated theoretically at various scales: microscopic scale (pore), macroscopic scale (laboratory, local), and domain scale.[1] Here, the macroscopic scale is defined as a representative element,[2] which is much larger than the microscopic scale but much smaller than the domain scale. In many situations, two or multiple scales coexist. In general studies, a model for the DRT processes in porous media is usually generalized by combining the transport equation (TE) with reducing to the Navier–Stokes equations (NSE) for porosity equal to 1 or to the earlier porous media models in the appropriate ranges of parameters.[3] In fact, the DRT process in porous media clearly requires some more sophisticated descriptions than that provided by continuum approaches, such as the relationship between the macroscopic DRT coefficients of porous media and their microscopic geometry,[4] the geometrical properties of interfaces,[5−8] and the relationship between the DRT coefficients and the morphology of the flow.[9,10]

Up to now, many analysts lead DRT processes in porous media to a system of nonlinear partial differential equations and ordinary differential equations with typically strongly varying coefficients;[11−13] in order to avoid a restriction of the time step caused by stability conditions, they must apply implicit schemes for the approximation of the time derivatives. In many practical problems, the investigation for DRT processes in porous media is often characterized by strongly local phenomena (such as marching fronts), and the adaptive numerical method with refined grids often needs to be used for the spatial discretization.[14−16] Though all these traditional methods can provide accurate results for DRT processes in porous media, they are not convenient, especially for processing the boundary conditions.

In recent years, as a new computational method, the lattice Boltzmann method (LBM) has been successfully set up for fluid flow in porous media [3,17] and has proven to be competitive. The LBM is based on discrete particle description of a fluid in porous media and provides many of the advantages of molecular dynamics such as clear physical pictures and allows us to define the complicated boundary conditions. In this Letter, we report a comprehensive study for the DRT processes in porous media that combines the LBM with the classical principle of porous flow. As a test of our method, we present an example for the case of DRT processes in heterogeneous porous media. The results agree well with the theoretic prediction.

In order to understand such a DRT system, we need an idea of how fluids flow in porous media. Here, we take the model proposed by Nithiarasu *at al.*[3] In this model, by considering the buoyancy driven flow in a two-dimensional rectangular cavity and applied for forced convective heat transfer through a variable porosity medium, the Navier–Stokes equation can be expressed as

$$\nabla \cdot \boldsymbol{v} = 0, \tag{1}$$

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$$\frac{\partial \boldsymbol{v}}{\partial t}+(\boldsymbol{v}\cdot\nabla)\Big(\frac{\boldsymbol{v}}{\phi}\Big)=-\frac{1}{\rho}\nabla(\phi P)+\nu_e\nabla^2\boldsymbol{v}+\boldsymbol{F}, \tag{2}$$

where ρ is the fluid density, P is pressure, ν_e is an effective parameter equated to the shear viscosity of fluid ν times the viscosity ratio J, and $\boldsymbol{F}$ represents the total body force due to the presence of the porous media and other external force fields, which can be expressed as

$$\boldsymbol{F}=-\frac{\phi\nu}{K}\boldsymbol{v}-\frac{\phi F_\phi}{\sqrt{K}}|\boldsymbol{v}|\boldsymbol{v}+\phi G, \tag{3}$$

where G is the body force induced by an external force. The geometric function F_ϕ and the permeability K are as follows:[18,19]

$$F_\phi=\frac{1.75}{\sqrt{150\phi^3}}, \tag{4}$$

$$K=\frac{\phi^3 d_p^2}{150(1-\phi)^2}, \tag{5}$$

where d_p is the solid particle diameter.

To obtain the capillary pressure–fluid content relationship, we define the reduced fluid saturation S as follows:

$$S=\frac{\theta-\theta_r}{\theta_s-\vartheta_r},\quad 0\le S\le 1, \tag{6}$$

where θ_r and θ_s denote the residual fluid content which remains even in the dry porous media and the fluid content of the saturated porous media, respectively. Considering the principle of chemical reaction dynamics and the idea of Ref. [12], we can derive a coupled TP system of a partial differential equation (PDE)

$$\frac{\partial(Sc_1)}{\partial t}-\nabla\cdot(SD\nabla c_1-\rho v c_1)+\lambda_1 S c_1^{n_1}c_2^{n_2}=0, \tag{7}$$

and an ordinary differential equation (ODE)

$$\frac{\partial c_2}{\partial t}+\lambda_2 c_1^{n_2}c_2^{n_1}=0, \tag{8}$$

where c_1 is the concentration of the mobile substance while c_2 is the concentration of immobile substance. D is the dispersion tensor and can be expressed as

$$\begin{aligned} D&=\begin{pmatrix} A_{11} & (\alpha_l-\alpha_t)(q_xq_y/|q|)\\ (\alpha_l-\alpha_t)(q_xq_y/|q|) & A_{22}\end{pmatrix},\\ A_{11}&=\alpha_l(q_x^2/|q|)+\alpha_t(q_y^2/|q|)+D_m,\\ A_{22}&=\alpha_t(q_x^2/|q|)+\alpha_l(q_y^2/|q|)+D_m, \end{aligned} \tag{9}$$

where $|q|=\sqrt{q_x^2+q_y^2}$and D_m is the molecular diffusion, which in most applications is much smaller than the dispersion and therefore usually neglected; α_l and α_t are the longitudinal and transverse dispersivities respectively. Here we neglect the dependence of the dispersivities on the saturation and choose $\alpha_t\approx 0.1\alpha_l$;[20,21] λ_1 and λ_2 are the two reaction rate constants, n_1 and n_2 are the two chemical equivalent constants.

Employing the above equations, we can conveniently study the DRT processes in porous media by first solving Eqs. (1) and (2), but it is not easy to obtain the solution for Eqs. (1) and (2) because the geometries of porous media are very complex. Due to the successful applications of the lattice Boltzmann computational technique in a complex flow field,[22–25] researchers have obtained several achievements for porous flow field.[1,2,26] We employ the statistical average principle, and the LBM scheme is expressed as

$$\bar f_i(\boldsymbol{x}+\boldsymbol{e}_i\delta_t,t+\delta_t)=\bar f_i(\boldsymbol{x},t)-\frac{\bar f_i(\boldsymbol{x},t)-\bar f_i^{eq}(\boldsymbol{x},t)}{\tau}+F_i\delta_t, \tag{10}$$

where δ_t is the time increment, $\bar f_i(\boldsymbol{x},t)$ and $\bar f_i^{eq}(\boldsymbol{x},t)$ are the volume-averaged distribution function and equilibrium distribution function at the representative elementary volume scale, respectively (in the following, the overbars will be omitted for the sake of convenience), τ is the relaxation time, and F_i is the force term for ith particle of fluid. For the $D2Q9$ model,[22] the discrete velocities are given by

$$\boldsymbol{e}_i=\begin{cases} 0, & \text{for}\quad i=0;\\ \Big(\cos\dfrac{(i-1)\pi}{2},\sin\dfrac{(i-1)\pi}{2}\Big), & \text{for}\quad i=1-4;\\ \sqrt{2}\Big(\cos\Big[\dfrac{(i-5)\pi}{2}+\dfrac{\pi}{4}\Big],\sin\Big[\dfrac{(i-5)\pi}{2}+\dfrac{\pi}{4}\Big]\Big), & \text{for}\quad i=5-8.\end{cases} \tag{11}$$

The equilibrium distribution function is

$$f_i^{eq}=A_i\rho\Big[1+\frac{\boldsymbol{e}_i\cdot\boldsymbol{v}}{RT}+\frac{(\boldsymbol{e}_i\cdot\boldsymbol{v})(\boldsymbol{e}_i\cdot\boldsymbol{v})}{2\phi(RT)^2}-\frac{\boldsymbol{v}\boldsymbol{v}}{2\phi RT}\Big], \tag{12}$$

where R is the gas constant and T the temperature of the fluid. The corresponding weight coefficients are $A_0=4/9$, $A_i=1/9$ $(i=1,2,3,4)$, $A_i=1/36$ $(i=5,6,7,8)$. According to Refs. [4,5], we obtain F_i as

$$F_i=A_i\rho\Big(1-\frac{1}{2\tau}\Big)\Big(\frac{\boldsymbol{e}_i\cdot\boldsymbol{F}}{RT}+\frac{(\boldsymbol{e}_i\cdot\boldsymbol{v})(\boldsymbol{e}_i\cdot\boldsymbol{F})}{\phi R^2T^2}-\frac{\boldsymbol{v}\cdot\boldsymbol{F}}{\phi RT}\Big). \tag{13}$$

The density and velocity of fluid are defined by

$$\rho=\sum_i f_i,\quad \boldsymbol{v}=\sum_i f_i\boldsymbol{e}_i/\rho+\frac{\delta_t}{2}\boldsymbol{F}. \tag{14}$$

The macroscopic equations for αth fluid flows in porous media may be recovered by a Taylor expansion and a Chapman–Enskog expansion, respectively, as follows:

$$\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho\boldsymbol{v})=0, \tag{15}$$

$$\frac{\partial(\rho \boldsymbol{v})}{\partial t} + \nabla \cdot \left(\frac{\rho \boldsymbol{v}\boldsymbol{v}}{\phi}\right) = -\nabla P + \nabla \cdot [\rho \nu_e (\nabla \boldsymbol{v} + \boldsymbol{v}\nabla)] + \boldsymbol{F}; \tag{16}$$

where $\nu_e = (\tau - 0.5)RT\delta_t$, and it is the same as in Eqs. (2) and (3). Noting that as $\phi = 1$, Eq. (16) will be reduced to the standard lattice Boltzmann equation for the fluid flows in the absence of porous media, another interesting fact is that Eq. (16) will be reduced to Darcy's law when the flow in porous media is very slow.

As a test of this method, we simulate the DRT processes in a heterogeneous porous medium. We consider a two-dimensional horizontal case, in which the influence of the gravitation is neglected, and the DRT process can be described as a strongly heterogeneous diagnostic test strip or a thin confined piece of soil with stochastically distributed properties in the horizontal direction only. The system of our present model is solved on a rectangular domain Ω with two short and two long sides facing each other:

$$\Omega = \{(x, y) \in \mathbb{R}^2 \mid 0 < x < 1,\ 0 < y < 5\}. \tag{17}$$

The reduced fluid saturation S, the concentrations of mobile substance c_1 and immobile substance c_2 are normalized and thus are within the interval [0, 1]:

$$0 \le S,\ c_1, c_2 \le 1. \tag{18}$$

The boundary conditions are designed as

$$S(x, y, t) = 1,\ y = 0, \tag{19}$$
$$e_n.\nabla S(x, y, t) = 0,\ y = 50, \tag{20}$$
$$e_n.\nabla S(x, y, t) = 0,\quad x = 0, \tag{21}$$
$$e_n.\nabla S(x, y, t) = 0,\quad x = 12.5, \tag{22}$$

where $e_n \in \mathbb{R}^2$ denotes the normal vector on the boundary $\partial\Omega$.

The mobile substance through the above boundaries is prohibited by the conditions

$$c_1(x, y, t) = 1,\quad y = 0, \tag{23}$$
$$e_n.\nabla c_1(x, y, t) = 0,\quad y = 50, \tag{24}$$
$$e_n.\nabla c_1(x, y, t) = 0,\quad x = 0, \tag{25}$$
$$e_n.\nabla c_1(x, y, t) = 0,\quad x = 12.5. \tag{26}$$

Because of Eqs. (20)–(22), the following equation:

$$e_n \cdot \rho v = e_n \cdot \frac{1}{n_e}\mathcal{D}(S)\nabla S = 0, \tag{27}$$

holds for all boundaries. The initial values are given by

$$S(x, y, 0) = 0,\quad y > 0, \tag{28}$$
$$c_1(x, y, 0) = 0,\quad y > 0, \tag{29}$$

$$c_2(x, y, 0) = \begin{cases} 1, & 14 + 0.7x < y < 22 + 0.7x; \\ 0, & \text{elsewhere.} \end{cases} \tag{30}$$

which provides an absolutely unsaturated porous media with a reaction zone.

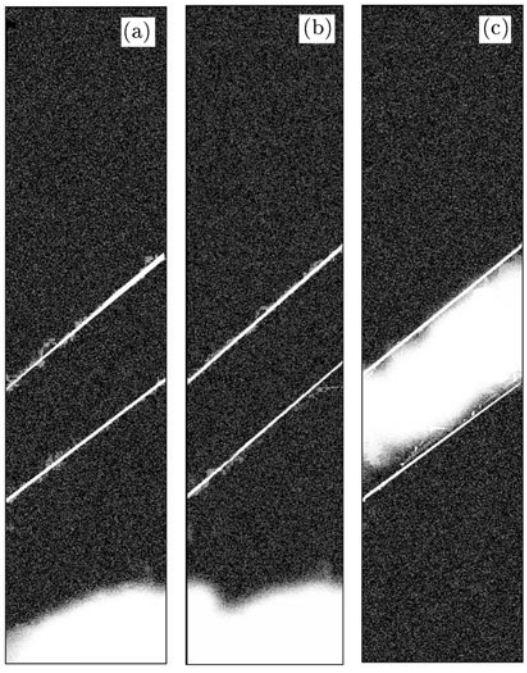

Fig. 1. Initial patterns: (a) reduced fluid saturation S, (b) concentration c_1, (c) concentration c_2.

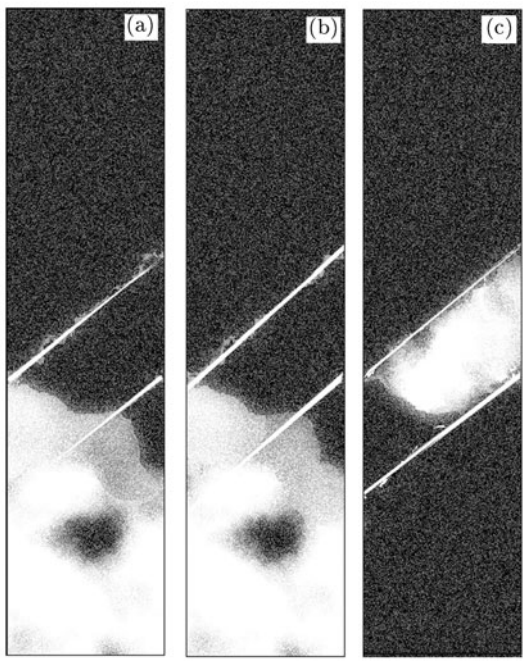

Fig. 2. Pattern for 171 time steps: (a) reduced fluid saturation S, (b) concentration c_1, (c) concentration c_2.

Using a visualization computing technique, the results are shown on Figs. 1–3. The left-hand sides of these figures present the reduced fluid saturation S

for different time, the middle of these figures present the concentration c_1 of the mobile substance, while the right-hand sides show the concentration c_2 of the immobile substance. For all pictures, white represents S, c_1, $c_2 = 1$, black represents S, c_1, $c_2 = 0$, all tiny grey points represent solid media, and the reaction zones are bounded by $14 + 0.7x < y < 22 + 0.7x$ with two white lines. Thus, according to the boundary conditions the liquid with a concentration c_1 of the mobile substance enters the porous media at the inflow-boundary. Because of the heterogeneity, some parts of the porous media remain dry for a long time, although the neighbourhood is already almost saturated. After a finite number of time steps (171 time steps), the liquids reaches the reaction zone which is set in Eq. (30). In this region, the concentration of the mobile phase decreases until the immobile substance is completely consumed. The steady-state solution, reached after approximately 240 time steps, is a totally saturated porous medium.

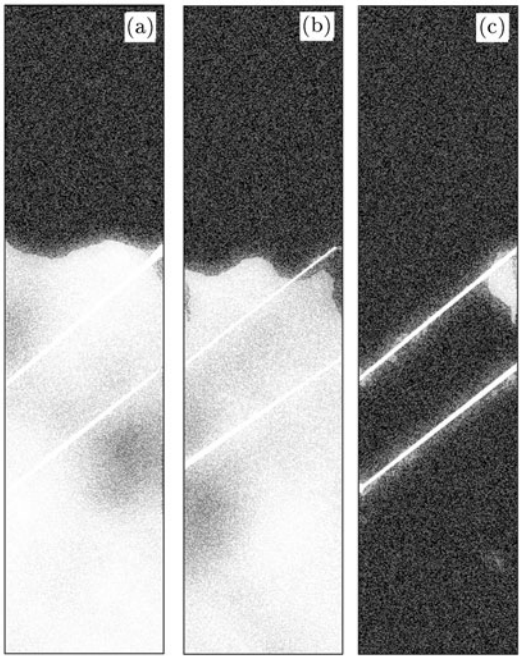

Fig. 3. Pattern for 240 time steps: (a) reduced fluid saturation S, (b) concentration c_1, (c) concentration c_2.

In conclusion, we should point out that for the DRT process in porous media, our model is more fundamental than previous ones, and the computational efficiency and stability are satisfactory. Hence it will be helpful for detailed study of the evolution of (DRT) processes in porous media.

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