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# A new method for simulation and analysis of displacement of fluids in porous media*

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Using the principle of diffusion-limited aggregation (DLA), a new model is introduced to simulate the displacement of one fluid by another in porous media. The results agree with experiments, apparently they do not leave out film-flow phenomena. Simultaneously, we also present a new numerical method to treat our results by the lattice Boltzmann method (LBM). All these will be helpful for analysing similar subjects.

**Keywords:** displacement in porous media, diffusion-limited aggregation (DLA), numerical treatment
**PACC:** 4755M, 6780, 0340G

## 1. Introduction

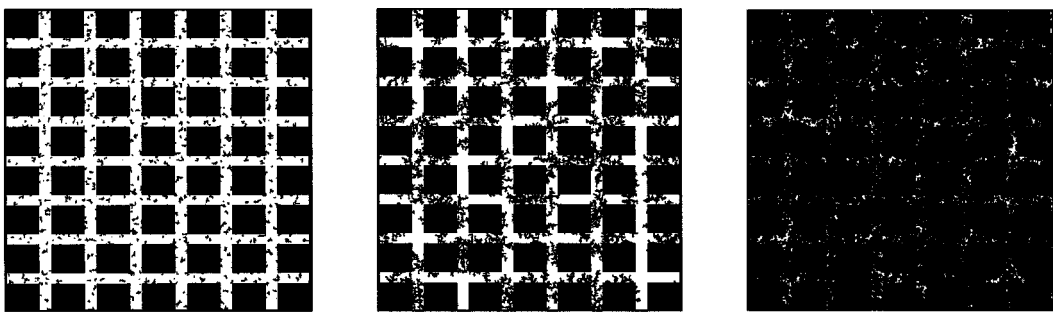
In recent years, the behaviour of the displacement in porous media has attracted considerable attention.[1,2] This is due to its important applications in petroleum recovery, gas production, packed-bed catalytic reactors, drying of porous solids, geothermal reservoirs, thermal insulation, packed-bed storage tanks, grain storage and others. In the literature, the number of works which present models to describe the displacement in porous media is very small. To the best of our knowledge, models for the displacement in porous media, similar to those considered in non-porous media, are difficult yet. The essential feature of these systems is that they comprise two interpenetrating phases, the pores and solid networks. Our ability to understand physical processes within these systems is often limited by the lack of suitable mathematical representation of their geometry. Existing models are usually restricted to the case in which the solid phase can be viewed as a packing of simple shaped grains.[3,4] But natural porous media tend to have a more intricate pore structure and a wider distribution of pore sizes. In this paper, we report a comprehensive study of the displacement processes in a broad range of porous media that combines diffusion-limited aggregation (DLA) principle[5−9] with computer modelling. We also present a procedure to better understand the underlying physics of this modelling by making use of the full information obtained in our previous investigations.[10,11]

## 2.Implementing the model and general survey

The DLA model was introduced by Witten and Sander firstly.[5] In this paper, we use it for simulating the displacement of one fluid by another in porous media. The schematic principle of the model is as follows: suppose there is a $464 \times 464$ lattice substrate of porous medium in which the pores are homo-distributed and the porosity $\varphi$ equals to 0.425(see Fig.1). Let us consider the process that a non-wetting fluid, say oil (shown black) which has been adsorbed on solid phase of the porous medium, is being displaced from the pore of the medium by a wetting fluid, say water (shown white). First, we suppose that a seed particle of oil is displaced by water, then it is deposited at the position $(x, y)$ and allowed to diffuse along four directions $(x \pm 1, y \pm 1)$ with equal probability until its diffu-

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sion steps reach $W$ (the maximum diffusion steps on the substrate). Then it is stopped, and becomes a nucleus of oil. Another particle of oil is displaced by water away from the origin, then it is launched and is allowed to walk at random (diffuse) until it arrives at a site adjacent to the nucleus of fluid, then it is also stopped. The third particle is as well displaced and launched and stopped adjacent to the two occupied sites, and so forth. In this way large clusters of fluid can be generated whose structure is expected to be characteristic for objects grown under diffusion-limited condition.



(a) Diffusion steps $W$=1000. (b) Diffusion steps $W$=6000. (c) Diffusion steps $W$=20000.

**Fig.1.** Displacement of one fluid by another in a homogeneous porous media. The non-wetting fluid, say oil, is shown black, the wetting fluid, say water, is white.

Fig. 1 shows a typical fluid cluster of 60 000 particles simulated by DLA. Figures 1 (a)–(c) represent the process at diffusion steps $W$ = 1000, 6000, and 20 000, respectively. In particular, Fig.1(c) shows the non-wetting fluid (say oil) is almost filling everywhere of pore space, which indicates that the displacement is almost finished. Indeed, this illustrates that the model in our paper can be used for simulating the displacement of one fluid by another in porous media. Let us consider the process that the capillary forces dominate the motion of the interface, the non-wetting fluid being displaced by the wetting fluid at a constant but very small flow rate. In this limit, the capillary forces show a strong inclination to dominate the displacements at the network of pores. Because the initial movement of interface is fast through the network of pores but becomes stuck later, so this process can be represented as a series of discrete jumps, and then the water displaces oil from the network of available pore at each time step.

Figure 1 also demonstrates the following two viewpoints: firstly, the pattern of displacement has a randomly branching, open structure; and secondly, the appearance of the pattern is stochastically self-similar, as in the case of fractals. Both points are due to the fact that the tips of most advanced branches capture the incoming diffusing fluid particles (suppose those are oil particles) most effectively. Thus, small fluctuations are enhanced, and this instability together with the randomness inherent in the model bring about a complex behaviour.[5,12]

In order to better understand the underlying physics of the above process, we give the following comments in terms of the lattice: (1) On every unit interval, a random number of particles of fluid (oil) are drawn from the uniform distribution and assigned to each site of a cell of linear size $L$. (2) Corresponding to the smallest capillary force, though the perimeter site is not selected randomly, a small random number of sites at a distance $r$ will be occupied. (3) The process of displacement starts with a seed particle and goes on by subsequent occupation of the perimeter sites. (4) Until the finite cell is filled completely, the process of displacement will not stop. (5) We study the structure of the region filled in by the invader fluid at this point by using a well defined configuration. (6) Suppose we have a parameter which is analogous to the occupation probability $p$ of ordinary percolation. In Fig.1, we can see that the pattern of the first displacements forms a connecting path between the two opposite edges of the cell. According to the Ref.[13], the number of sites occupied by the invader fluid at this moment can be expressed as $N \sim L^D$, where $N$ is the actual number of already occupied sites, $D \simeq 1.89$ in two dimensions. In this paper, because the fluids are incompressible, so an additional rule must be considered: for a region filled by "defender" sites, once it has been surrounded by the invading fluid, none of the sites belonging to this "trapped" area is available for occupation by the invading fluid, and in this case

the fractal dimension of the pattern of displacement is found to be $D \simeq 1.82$ (Fig.1). This value is different from that of Ref.[13]. In an analogy with static percolation, we can also define the defender cluster size distribution $n_s$ as follows:[14]

$$n_s \sim n_0(L)s^{-\tau}, \tag{1}$$

where $s$ is the number of the defender particles, $n_0(L)$ is the prefactor which scales with $L$, and the factor $\tau < 2$ has been shown to be the consistent value. This behaviour can be interpreted by the following mechanism: when one particle of fluid goes to a large cell, some of the smaller isolated clusters may turn out to be connected through parts which were outside of the original cell, and from larger clusters. Consequently, when $L$ increases, there is a net decrease in the density of clusters of a given size.

## 3. Numerical treatment

In order to help the analysis of displacement in the above model, let us review and extend the principle of fluid dynamics. We know that the motion of fluids through a porous medium like that shown in Fig.1 is governed by Darcy's law[15]

$$\boldsymbol{v}(x,y) = -K_i[\nabla \boldsymbol{p}(x,y) - \rho_i \boldsymbol{g}]. \tag{2}$$

Here $i = 1, 2$ labels the different fluids, $\rho_i$ is the density, and the constant $K_i$ is given in terms of the fluid viscosity $\mu_i$ and the crevice thickness of pore $b$ as[14]

$$K = b^2/12\mu_i, \tag{3}$$

while $\boldsymbol{g}$ is the component of the gravitational acceleration. For future discussion, we suppose that the fluids are incompressible and then introduce a complex potential function such that $w = \phi + \mathrm{i}\,\psi$. It is an analytic function of $z = x + \mathrm{i}\,y$, where the velocity potential $\phi = -\dfrac{k}{\mu}\boldsymbol{p}$ satisfies Laplace's equation $\nabla^2\phi = 0$, and the stream function $\psi$ will play a central role in the following analysis. Equations (2) and (3) constitute the Darcy approximation. They are derived in a series of ways from the Navier–Stokes equation by considering a parabolic flow profile parallel to the plates with a velocity that vanishes at both plates. On the other hand, the lattice Boltzmann method (LBM) is a new numerical method for the solution of the Navier–Stokes equations.[16–19] It has been discussed so far only in hydrodynamics. Its extension to fluid flow through porous media is straightforward.[2,10,11,20] In this paper, we use the prototype LBM model, which is implemented on a $64 \times 64$ D2Q9 lattice with one rest and eight moving particles.[21] The following discrete analogue of the BGK equation,

$$\begin{aligned} &F_{pi}(\boldsymbol{x} + \boldsymbol{c}_{pi}, t+1) \\ =&F_{pi}(\boldsymbol{x}, t) - \omega[F_{pi}(\boldsymbol{x}, t) - F^{\mathrm{e}}_{pi}(\boldsymbol{x}, t)], \end{aligned} \tag{4}$$

is solved on a regular lattice on which the set of particle density $F_{pi}(\boldsymbol{x}, t)$ is distributed. Here $F_{pi}$ is the average density of particles with velocity $\boldsymbol{c}_i$, $t$ is the time, $\boldsymbol{x}$ is the position vector of a node on the lattice, and $\omega$ is the relaxation parameter, which can be freely adjusted between 0 and 2. A generic choice for the equilibrium population $F^{\mathrm{e}}_{pi}(\boldsymbol{x}, t)$ is

$$\begin{aligned} F^{\mathrm{e}}_{pi} =& t_p \rho \Bigg[1 + \frac{\boldsymbol{c}_{pi\alpha}\boldsymbol{u}_\alpha}{c_{\mathrm{s}}^2} \\ &+ \frac{\boldsymbol{u}_\alpha \boldsymbol{u}_\beta}{2c_{\mathrm{s}}^2}\left(\frac{\boldsymbol{c}_{pi\alpha}\boldsymbol{c}_{pi\beta}}{c_{\mathrm{s}}^2} - \boldsymbol{\delta}_{\alpha\beta}\right)\Bigg], \end{aligned} \tag{5}$$

where $\alpha$ and $\beta$ are subscripts for the Cartesian components of the particle velocity. The hydrodynamic velocity is $\boldsymbol{u}_\alpha$, and density is $\rho$. The subscript $p$ is equal to the square of the modulus of the particle velocity $\boldsymbol{c}_{pi\alpha}$ and has been used to distinguish between velocities having different moduli. The subscript $i$ denotes the different velocities in the same speed class $p$. The constant $c_{\mathrm{s}}$ is proportional to a weighted average of the $\boldsymbol{c}_{pi\alpha}$ and is identified as the speed of sound in the model. Finally, $t_p$ is a weighting factor, which depends on $p$ and is adjusted to obtain isotropic fourth-order tensor products of $c_{pi\alpha}$ and to ensure Galilean invariance of the dynamics. The choice of Eq.(5) for the equilibrium population, when used together with Eq.(4), can be shown to lead to macrodynamic equations when truncated after the second-order in $\boldsymbol{u}_\alpha$, similar to the Navier–Stokes equations.[22] In the following we define the mass density $\rho$ by

$$\rho(\boldsymbol{x}, t) = \sum_{p,i} F_{pi}(\boldsymbol{x}, t), \tag{6}$$

and the hydrodynamic velocity $\boldsymbol{u}_\alpha$ by

$$\rho \boldsymbol{u}_\alpha = \sum_{p,i} F_{pi}\boldsymbol{c}_{pi\alpha}. \tag{7}$$

We introduce the quantity

$$\rho_1 = \sum_{p,i} F_{1pi}, \tag{8}$$

which may be thought of as the mass density of a component species whose particle density is $F_{1pi}$. The

dependence of $F_{pi}, F_{1pi}, \boldsymbol{u}_\alpha$ and $\rho_1$ on $x$ and $t$ is implied for notational convenience and will be implied henceforth. The variable corresponding to the granular degree is defined as

$$\Gamma = \frac{\rho_1}{\rho}, \tag{9}$$

where it is noted that, unlike the case of a true concentration variable, no constraint will be placed on the magnitude of $\rho_1$ and relative to $\rho$ and thus $\Gamma$ may take all values greater than zero.

By taking large scale averages from the lattice, the full Navier–Stokes equations may be approximated by a Chapman–Enskog series expansion

$$\partial_t \rho + \partial_\alpha(\rho \boldsymbol{u}_\alpha) = 0, \tag{10}$$

and

$$\begin{aligned} &\partial_t(\rho \boldsymbol{u}_\alpha) + \partial_\beta(\rho \boldsymbol{u}_\alpha \boldsymbol{u}_\beta) \\ &= -\partial_\alpha(\rho\Gamma) + \partial_\beta[\eta\partial_\beta(\rho \boldsymbol{u}_\alpha) + \eta\partial_\alpha(\rho \boldsymbol{u}_\beta)], \end{aligned} \tag{11}$$

where

$$\eta = \frac{c_s^2}{2}\left(\frac{2}{\omega} - 1\right) = \frac{\sqrt{\pi}}{8}\sigma\sqrt{\Gamma}. \tag{12}$$

Here $\sigma$ should be given in units of the lattice constant.

In porous media, solid bodies in the computation are represented by the set of nodes of the grid located inside the bodies. Two different types of boundary conditions are usually used. The first is a bouncing-back of the distribution function in the "rigid" nodes.[23] The second is to set the distribution function in the "rigid" boundary nodes equal to the equilibrium distribution function with zero velocity and density extrapolated from the flow and includes boundary nodes in the relaxation procedure of Eq.(4).[23] In this paper, we adopt the scheme for treating boundary condition by the method based on the Ref.[23]: a robust, second-order accurate treatment for the distribution function $F_{pi}$ on the boundaries is evaluated using Eq.(4), and the Taylor series expansion in both space and time for $F_{pi}$ near the wall. While maintaining a second-order accuracy of the solution in handling curved walls, the result indicates that the computational stability is improved.

Calculations with a stream function are more complicated because the prior streamline profile on the surface of the pattern of displacement is unknown. In this paper, we use the model described in the previous to compute solution of the stream function for the following reality example: a non-wetting fluid (say oil) which adsorbed on solid phase of a $464 \times 464$ square substrate of porous medium, and a wetting fluid (say water) is bounded by the pore and solid networks. Suppose the temperature and density are initially homogeneous for an unforced flow, $\sigma = 0.05$. In a first attempt, we choose the same fixed streamline profile at surface as for the configuration without a stream function. For a fully realistic calculation one has to include radiation from the surface in the program. We have performed a calculation with addition of stream function. In this case we have set the stream function in the whole streamline to a constant stream function ($\psi = 0.1$). The stream function at the boundary of porous medium is $\psi = 0$. The calculation without additional stream function converged after 7500 iterations towards a steady-state solution (see Fig.2).

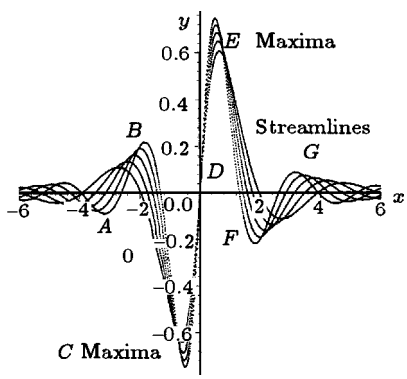



**Fig.2.** Evolution of the stream function $\psi$ for a configuration of the displacement of one fluid by another in a homogeneous porous media by lattice Boltzmann method.

We have seen that the qualitative features of Fig.2 can be understood under rather general circumstances on the basis of this paper. The most interesting feature is the generation of one extra pair of maxima and minima of $\psi$ which is denoted by $C$ and $E$ in the figure. Besides this, other points $A$, $B$, $F$, $G$ occur near the left and right edges. All these points represent that normal velocity $v_n = 0$. In order to be true extremum/saddle-point pairs of $\psi(x, y)$, the tangential velocity components at both sides of the interface at those points must have opposite direction. This can be decided by direct computation of the flow field in their neighbourhood. According to the above discussion, it is concluded that the extrema of $\psi$ are indeed an extremum/saddle-point pair. Similar arguments imply that the saddle-point cannot immediately abandon the interface. According to the above analysis, two important consequences have been obtained: (1) the mechanism of the DLA pattern is responsible for the displacement toward the stationary state at the

saddle-point, and (2) there exists an additional mechanism for the creation of new seed particle of oil displaced by water, and it is associated with the pinching-like morphology. In addition, our result is found in the same range as the results found in Refs.[5,24], but our method is obviously simpler and more convenient.

## 4. Summary and discussion

In summary, we have studied the displacement in porous media through binary fluids with fixed filler particles. Our results show that the domain growth can be significantly slowed down at late stages and qualitatively supports the previous studies.[2,6−11] The stream function distribution in a specimen used for the growth of displacement has been calculated using the lattice Boltzmann method. Our experiences show that the lattice Boltzmann method is a favourable tool for the calculation of the stream function distribution in an equipment used for the displacement of one fluid by another in porous media. It is expected that the displacement process can be incorporated on a microscopic scale and that the coupling between displacement and streamline can be studied in detail. We expect that new numerical evidence in the region of interface viscosity contrast may help to develop approximate schemes for the dynamics of displacement on the nonlinear dynamics of interface.

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