Lattice Boltzmann simulation of a multicomponent viscous fingering instability at high Schmidt number

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Introduction

The simulation of the multicomponent viscous fingering instability in the case of miscible fluids at high Schmidt number is investigated. This instability, firstly highlighted by Saffman & Taylor, occurs when a fluid of low viscosity moves into a fluid of higher viscosity. For this study, the mixing dynamics of two miscible components A and B of **equal molar mass** is simulated using a lattice Boltzmann model at the pore scale and, for a first attempt, at the representative volume.

Lattice Boltzmann multicomponent model

The lattice Boltzmann equation for species A can be written as:

$$f_\alpha^{\mathrm{A}}(\mathbf{x}+\mathbf{e}_\alpha\delta t, t+\delta t) - f_\alpha^{\mathrm{A}}(\mathbf{x},t) = \Omega_\alpha^{\mathrm{AA}}(\mathbf{x},t) + \Omega_\alpha^{\mathrm{AB}}(\mathbf{x},t)$$

Where Ω_α^{AA} and Ω_α^{AB} are respectively the **self-collision** term and the **cross-collision** term based on the kinetic theory proposed by **Sirovich** [1] and further adopted by Luo & Girimaji [2].

$$\Omega_\alpha^{\mathrm{AA}} = -s_{\mathrm{A}}\left(f_\alpha^{\mathrm{A}} - f_\alpha^{\mathrm{A}(0)}\right)$$
$$\Omega_\alpha^{\mathrm{AB}} = -\frac{1}{\tau_D}\frac{\rho_{\mathrm{B}}}{\rho}\frac{f_\alpha^{\mathrm{A}(eq)}}{c_s^2}(\mathbf{e}_\alpha - \mathbf{u})\cdot(\mathbf{u}_{\mathrm{A}} - \mathbf{u}_{\mathrm{B}})$$

ρ and $\mathbf{u}$ are respectively the barycentric density and velocity of the mixture. The mass density and velocity for each species are calculated from the distribution functions:

$$\rho_{\mathrm{A}} = \sum_\alpha f_\alpha^{\mathrm{A}} = \sum_\alpha f_\alpha^{\mathrm{A}(0)}$$
$$\rho_{\mathrm{A}}\mathbf{u}_{\mathrm{A}} = \sum_\alpha \mathbf{e}_\alpha f_\alpha^{\mathrm{A}} = \sum_\alpha \mathbf{e}_\alpha f_\alpha^{\mathrm{A}(0)}$$
$$\rho = \rho_{\mathrm{A}} + \rho_{\mathrm{B}}$$
$$\rho\mathbf{u} = \rho_{\mathrm{A}}\mathbf{u}_{\mathrm{A}} + \rho_{\mathrm{B}}\mathbf{u}_{\mathrm{B}}$$

The equilibrium function $f_\alpha^{A(0)}$ has the following form:

$$f_\alpha^{\mathrm{A}(0)} = \left[1 + \frac{1}{c_s^2}(\mathbf{e}_\alpha - \mathbf{u})\cdot(\mathbf{u}_A - \mathbf{u})\right] f_\alpha^{\mathrm{A}(eq)}$$

$$f_\alpha^{\mathrm{A}(eq)} = \omega_\alpha\rho_{\mathrm{A}}\left[1 + \frac{\mathbf{e}_\alpha\cdot\mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_\alpha\cdot\mathbf{u})^2}{2c_s^2} - \frac{\mathbf{u}\cdot\mathbf{u}}{2c_s^2}\right]$$

In order to improve the stability of the model, a **multiple relaxation time** framework is only applied on the self collision term. $\Omega_\alpha^{\mathrm{AA}}$ is rewritten as:

$$M^{-1}S^{\mathrm{A}}(\mathcal{M}^{\mathrm{A}(0)} - \mathcal{M}^{\mathrm{A}})$$

In two dimensions with nine velocity sets ($D2Q9$), moments and relaxation rates are defined by:

$$\mathcal{M}^{\mathrm{A}} = (\rho_{\mathrm{A}}, e_{\mathrm{A}}, \epsilon_{\mathrm{A}}, \rho_{\mathrm{A}}u_{x_{\mathrm{A}}}, q_{x_{\mathrm{A}}}, \rho_{\mathrm{A}}u_{y_{\mathrm{A}}}, q_{y_{\mathrm{A}}}, p_{xx_{\mathrm{A}}}, p_{xy_{\mathrm{A}}})$$
$$S^{\mathrm{A}} = diag\left(0, s_e^{\mathrm{A}}, s_\epsilon^{\mathrm{A}}, 0, s_q^{\mathrm{A}}, 0, s_q^{\mathrm{A}}, s_\nu^{\mathrm{A}}, s_\nu^{\mathrm{A}}\right)$$

Finally a Chapmann-Enskog expansion shows that the model recovers the Navier-Stokes equations for the mixture and the **Fick's law** for binary diffusion. Relations between the relaxation rates and the kinematic viscosity ν^{A}, bulk viscosity $\nu_{\mathcal{B}}^{\mathrm{A}}$, and the diffusion coefficient D^{AB} are obtained as:

$$\nu^{\mathrm{A}} = \frac{1}{3}\left(\frac{1}{s_\nu^{\mathrm{A}}} - \frac{1}{2}\right), \quad \nu_{\mathcal{B}}^{\mathrm{A}} = \frac{2}{9}\left(\frac{1}{s_e^{\mathrm{A}}} - \frac{1}{2}\right), \quad D^{\mathrm{AB}} = \frac{1}{3}\left(\tau_D - \frac{1}{2}\right)$$

s_q^{A} is taken as $8\frac{2-s_\nu^{\mathrm{A}}}{8-s_\nu^{\mathrm{A}}}$ in order to improve the bounce-back precision [3] and other relaxation rates are set to s_ν^{A}.

Numerical simulation

A flow with a low enough velocity through a porous medium follows the **Darcy's law**: $-\nabla P = \frac{\nu}{K}v$. Following the work of Dong et al.[4] for immiscible fluids, we compare the influence of the viscous ratio $M = \nu^{\mathrm{B}}/\nu^{\mathrm{A}}$ at the **pore scale** but for miscible components at high Schmidt number $Sc = \nu^{\mathrm{A}}/D^{\mathrm{AB}}$. Grid and boundary conditions are presented in figure 1. The permeability of the porous medium is calculated: $K = 44$ LU (see figure 2).

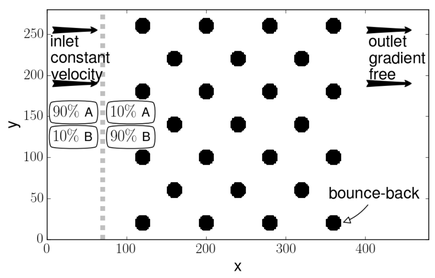


Figure 1: Grid, initial and boundary conditions

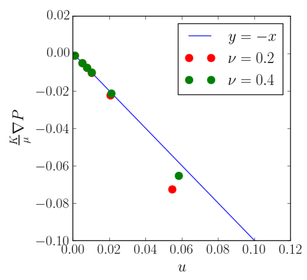


Figure 2: Darcy law validation

- As expected the Darcy's law is only valid for low speed flow. Outside of this range, the Darcy–Forchheimer law should be used.
- For low viscosity ratio, thin patterns rise between pores and reach the outlet at the same time.
- For larger viscosity ratio, patterns tend to enlarge due to the higher viscosity of the displaced fluid near the pores.
- These observations do not exhibit any particular finger structure at pore scale suggesting that viscous fingering can only be triggered at a much larger scale.

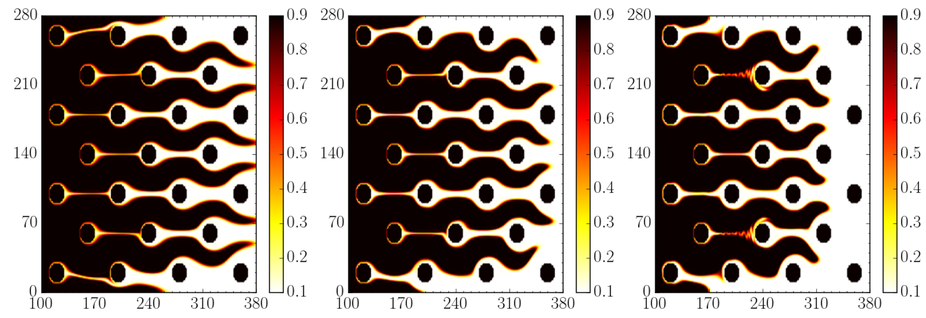
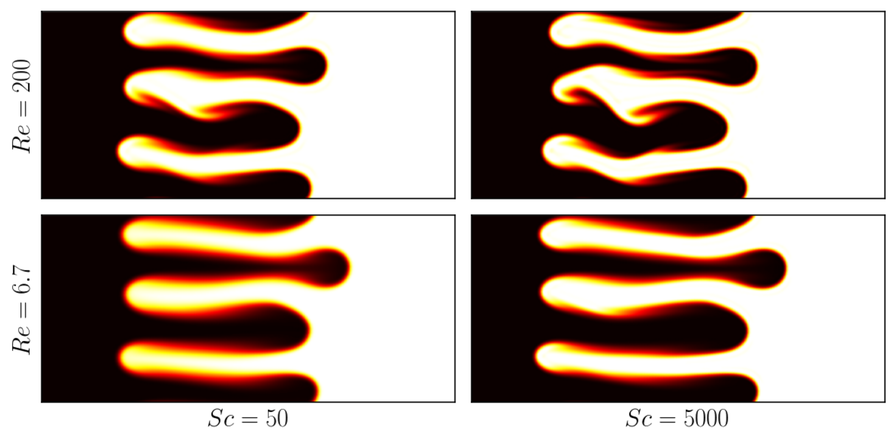


Figure 3: $tstep = 4500$ for different viscosity ratios ($M = 1, 5, 10$) at $Sc = 5000$

Current work: from pore scale to representative volume

- Grey lattice Boltzmann model [5]: $f_\alpha^{coll} = (1 - n_s)\times Coll + n_s \times f_{opp}$
- $n_s^{\mathrm{A}}[i,j] = \nu^{\mathrm{A}}/\left(2K[i,j] + \nu^{\mathrm{A}}\right)$
- Random permeability field ($K_{mean} = 39$ LU)
- $M = 10$, $U_0 = 0.01$
- $Re = U_0 N_y/\nu^{\mathrm{A}}$



Perspectives

- Different molar mass: interpolation or modification of the equilibrium
- Three and more species: the Maxwell-Stefan equations
- MRT model for the cross-collision term as Asinari's previous works [6]
- Chemical reactions: source/sink terms and temperature

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