Lattice Boltzmann model for miscible mixtures: application to the viscous fingering instability

Lucien Vienne, S. Marié & F. Grasso

Laboratoire DynFluid, Arts et Métiers ParisTech, France
Conservatoire National des Arts et Métiers, France

Objective: Saffman-Taylor instability

2 miscible species + different viscosity + porous medium

Challenge

Simulation of miscible viscous fingering instability by the LBM

Questions:
- ↪ Multi-species with LBM?
- ↪ Porous medium with LBM?
- ↪ Viscous fingering with 3 species?

Multiple species using LBM

an inter-molecular friction force

Multi-species using LBM

Species distribution functions

$$f_\alpha^m(\mathbf{x}, t)$$

↪ Each species m has its own distribution function which is governed by its own kinetic equation.

$$\rho_m = \sum_\alpha^{D2Q9} f_\alpha^m,$$

$$\rho_m \mathbf{u}_m = \sum_\alpha^{D2Q9} f_\alpha^m \mathbf{e}_\alpha$$

- Single species: BGK collision operator
- Mixture: no unique/well-established relaxation collision operator
- Different LB models depending on the underlying kinetic theory (collision is modified): *Luo and Girimaji 2003; Asinari 2006-2008; Arcidiacono et al. 2007*

↪ Diffusion interaction among species is taken into account by the means of a force. Since collision is not altered, this method can easily be introduced in any other LB algorithm.

Multi-species using LBM

Part 1: viscosity

$$f_\alpha^m\left(\mathbf{x}+\mathbf{e}_\alpha\delta_t, t+\delta_t\right) = f_\alpha^m\left(\mathbf{x},t\right) - \frac{1}{\tau_m}\left[f_\alpha^m\left(\mathbf{x},t\right) - f_\alpha^{m(eq)}\left(\mathbf{x},t\right)\right]$$

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Wilke's formula

$$\mu_m = \rho_m c_s^2(\tau_m - \frac{\delta_t}{2}), \quad \mu_m = \frac{x_m \mu_{0,m}}{\sum_n^N x_n \Phi_{mn}}$$

$$\Phi_{mn} = \frac{1}{2\sqrt{2}}\left(1+\frac{M_m}{M_n}\right)^{-\frac{1}{2}}\left[1+\left(\frac{\mu_{0,m}}{\mu_{0,n}}\right)^{\frac{1}{2}}\left(\frac{M_n}{M_m}\right)^{\frac{1}{4}}\right]^2$$

Multi-species using LBM

Part 2: inter-molecular friction force

$$f_\alpha^m\left(\mathbf{x}+\mathbf{e}_\alpha\delta_t, t+\delta_t\right) = f_\alpha^m\left(\mathbf{x},t\right) - \frac{1}{\tau_m}\left[f_\alpha^m\left(\mathbf{x},t\right) - f_\alpha^{m(eq)}\left(\mathbf{x},t\right)\right] + S_\alpha^m\left(\mathbf{x},t\right)$$

↪ Each species m has its own distribution function which is governed by its own kinetic equation.

$$\rho_m = \sum_\alpha^{D2Q9} f_\alpha^m,$$

$$\rho_m \mathbf{u}_m = \sum_\alpha^{D2Q9} f_\alpha^m \mathbf{e}_\alpha + \frac{\delta_t}{2}\mathcal{F}_m$$

Inter-molecular friction force

$$\mathcal{F}_{D,m} = -p\sum_{n=1}^{N}\frac{x_m x_n}{\mathcal{D}_{mn}}(\mathbf{u}_m - \mathbf{u}_n)$$

Maxwell 1867; *Chapman and Cowling 1932*; *Hirschfelder, Curtiss, and Bird 1954*; *Kerkhof and Geboers 2004*

- S_α^m: Guo's forcing source term (*Guo, Zheng, and Shi 2002*)
- $\mathcal{D}_{mn}$: Maxwell-Stefan diffusion coefficient

Multi-species using LBM

Part 2: inter-molecular friction force

$$f_\alpha^m\left(\mathbf{x}+\mathbf{e}_\alpha\delta_t, t+\delta_t\right) = f_\alpha^m\left(\mathbf{x},t\right) - \frac{1}{\tau_m}\left[f_\alpha^m\left(\mathbf{x},t\right) - f_\alpha^{m(eq)}\left(\mathbf{x},t\right)\right] + S_\alpha^m\left(\mathbf{x},t\right)$$

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↪ Validated on binary diffusion, ternary diffusion (included multicomponent effects), and convection-diffusion problems. (*submitted Vienne and Marié 2019*)

Porous medium using LBM

two strategies for a volume averaging approach

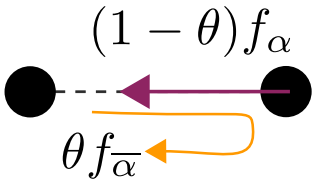
Porous medium using LBM

1st strategy - gray lattice Boltzmann (GLBM), *Yoshida and Hayashi 2014*

Gray lattice Boltzmann strategy: porous medium effect $\sim$ partial bounce-back

- θ is the amount of reflection

$$\theta_m = 0 \Rightarrow \text{ standard streaming}$$
$$\theta_m = 1 \Rightarrow \text{ bounce-back condition}$$



- θ is defined on the link between lattice nodes

$$\frac{\mu_m}{K\rho_m} = \frac{2\theta_m}{(1-\theta_m)\delta_t}$$ with K permeability of the porous medium

Porous medium using LBM

2nd strategy - Brinkman forcing scheme (BF), *Ginzburg 2008*

Porous medium effect $\sim$ global drag effect:

$$\mathcal{F}_{porous,m} = -\frac{\mu_m}{K}\mathbf{u}_m$$

Note : For both GLBM and BF schemes, the numerical permeability depends lightly on the relaxation time. We use the MRT collision model (*d'Humières et al. 2002*) with $\Lambda = 3/16$ (TRT) corresponding to $s_q = 8\frac{2-1/\tau_m}{8-1/\tau_m}$.

Simulation of miscible viscous fingering instability by the LBM

Multi-species with LBM ✓
↪ inter-molecular friction force

Porous medium with LBM ✓
↪ 2 strategies: GLBM and BF schemes

Viscous fingering

Viscous fingering

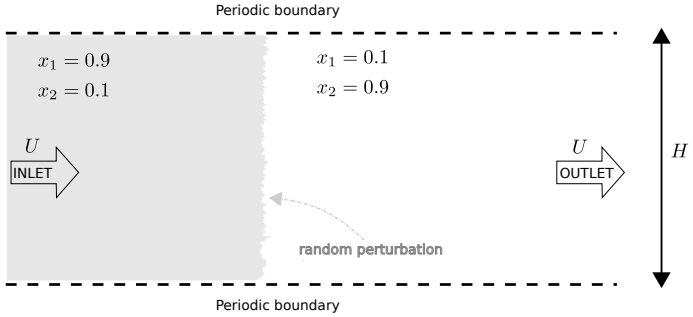
This interfacial instability occurs when a less viscous fluid displaces a more viscous fluid in a porous medium.

- Mixing in porous media is particularly difficult due to the absence of inertia
- but it plays a key role in carbon sequestration, oil recovery, mantle convection, microfluidic device, chromatographic columns, and proton exchange membrane fuel cell.

Viscous fingering (*Homsy 1987*).

Viscous fingering

Initial conditions



Initial conditions

$$f_\alpha^m(t=0) = f_\alpha^{m(eq)}(\rho_m, u_{x,m} = U, u_{y,m} = 0)$$

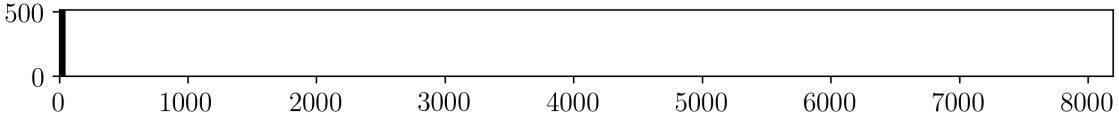
Dimensionless numbers

$$R = \ln\left(\mu_{0,2}/\mu_{0,1}\right) = 3$$

$$P_e = \frac{UH}{\mathcal{D}_{12}} = [500...16000]$$

Viscous fingering

Global dynamics



$R = 3, \quad P_e = 2000.$

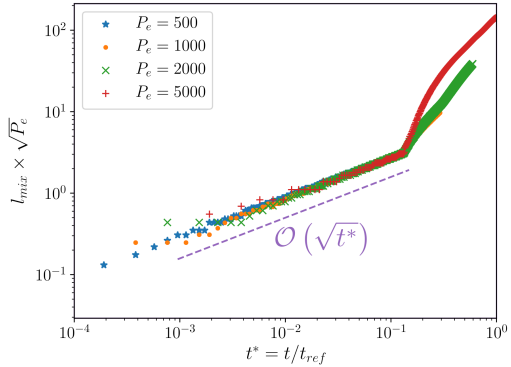
- Coarsening of the fingers in the transverse direction.
- Growth of the fingers in the streamwise direction

Viscous fingering

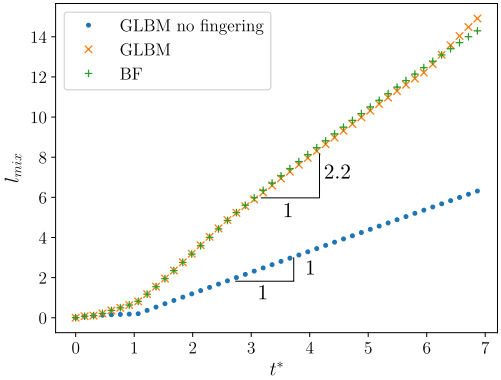
Mixing length

Mixing length

$$l_{mix}(t) = ||\bar{X}_{0.899}(t) - \bar{X}_{0.101}(t)||$$



$R = 3$, $t^* = t/t_{ref} = t \times U/H$.

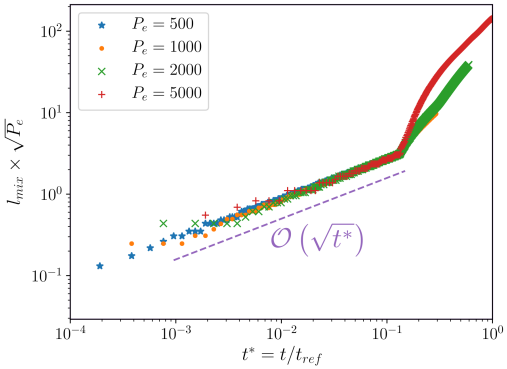


$R = 3$, $Pe = 2000$, $t^* = t/t_{ref} = t \times U/H$.

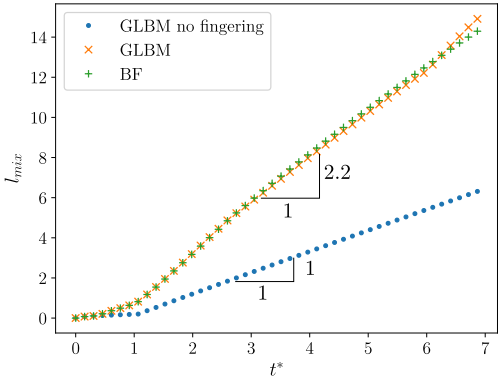
Viscous fingering

Mixing length

- Diffusion dominated regime for $t^* < 0.1$
- Advection dominated regime for $t^* > 1$
- No difference between GLBM and BF schemes



$R = 3$, $t^* = t/t_{ref} = t \times U/H$.



$R = 3$, $Pe = 2000$, $t^* = t/t_{ref} = t \times U/H$.

Viscous fingering

Early times

Assuming a perturbation

$$x'_m(\mathbf{x}, t) = x'_m(\mathbf{x}) \exp(\sigma t)$$

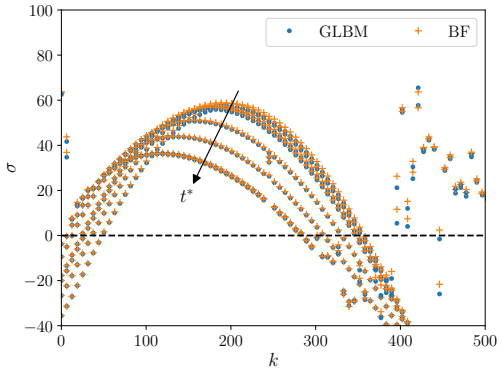
Growth rate of the perturbation σ

$$\begin{aligned} x'_m(\mathbf{x}, t) &= x^0_m(\mathbf{x}, t) - x_m(\mathbf{x}, t) \\ \hat{x}(x, k, t) &= \mathsf{FFT}_y\left(x'_m(\mathbf{x}, t)\right) \\ a(k, t) &= ||\hat{x}(x, k, t)||_2 = \sqrt{\int_0^{n_x} \hat{x} \cdot \hat{x} dx} \\ \sigma(k, t) &= \frac{d \ln\left(a(k, t)\right)}{dt} \end{aligned}$$

x^0_m: base state $\Longleftrightarrow$ non-perturbed simulation.

Viscous fingering

Influence of the porous model

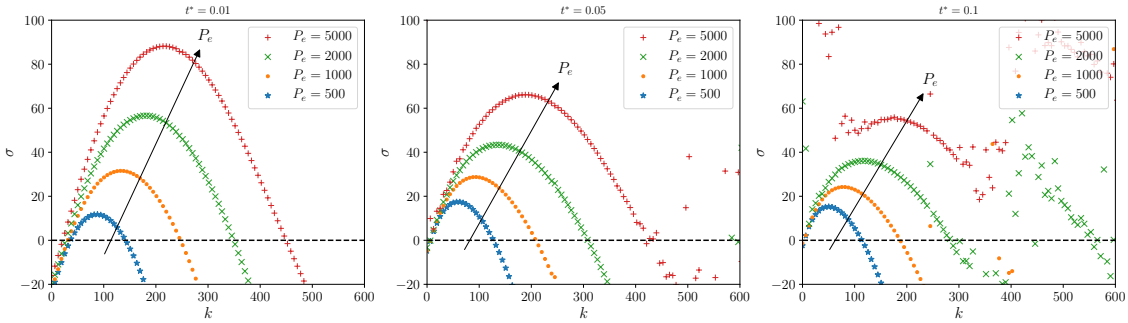


Dispersion curves for $R = 3$, $P_e = 2000$ at various times $t^* = t/t_{ref} = t \times U/H$.

- GLBM and BF schemes leads to equivalent growth rates.
- Growth rate decreases in time.
- Most dangerous, threshold and cutoff wave numbers are reduced as the instability progresses.

Viscous fingering

Influence of the Péclet number $P_e = \frac{UH}{\mathcal{D}_{12}}$



Dispersion curves for $R = 3$ at $t^* = 0.01,\ 0.05,\ 0.1$ with different Péclet values.

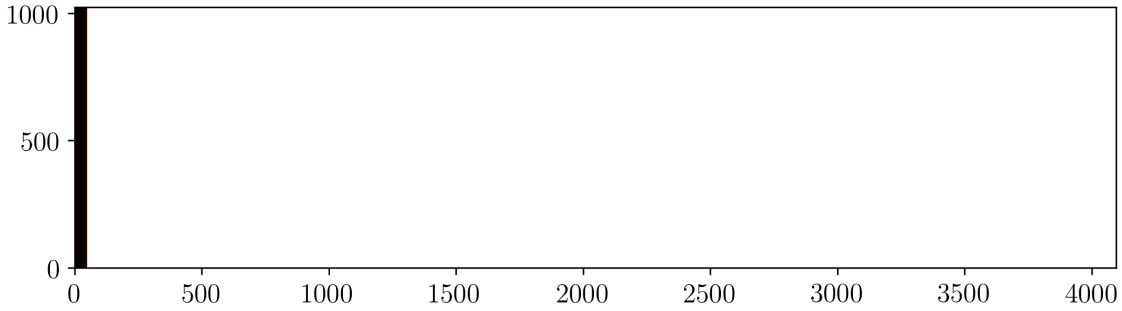
- High Péclet numbers lead to a more intense instability.
- The range of unstable wave numbers and the growth rate increase with P_e.
- The Péclet number influences the transition from linear to non-linear interactions.

Viscous fingering

Intermediate times

Non-linear interactions

- spreading, shielding, fading, coalescence
- tip splitting, and side branching



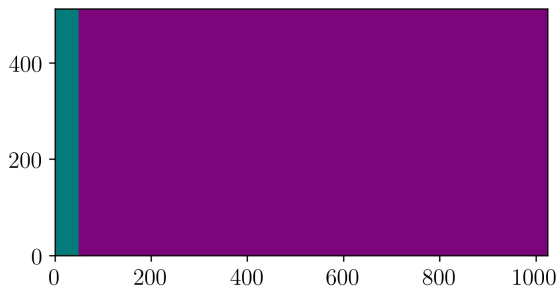
$R = 3, \quad P_e = 16000.$

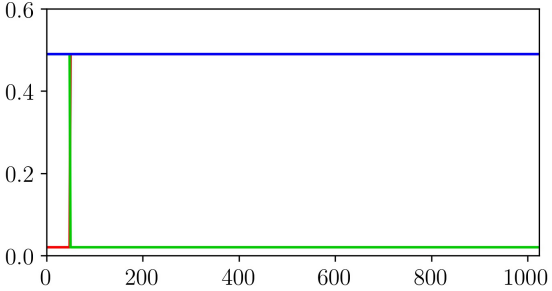
Ternary mixture & viscous fingering

multicomponent effects

Viscous fingering

3 species - stable configuration, no fingering





3 species → RGB channels

$$\left.\begin{aligned} x_1 &= 0.02\ R \\ x_2 &= 0.49\ G \\ x_3 &= 0.49\ B \end{aligned}\right\} \quad \left.\begin{aligned} x_1 &= 0.49\ R \\ x_2 &= 0.02\ G \\ x_3 &= 0.49\ B \end{aligned}\right\}$$

Pure viscosity

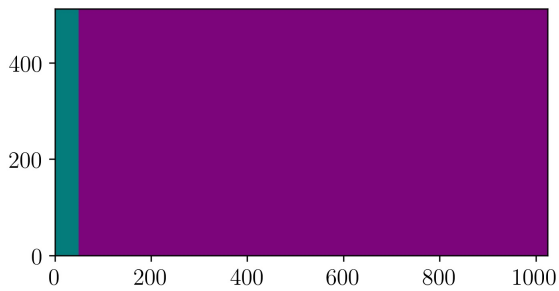
$$\mu_{0,1} = 0.5 \text{ [lu]}$$
$$\mu_{0,2} = 0.5 \text{ [lu]}$$
$$\mu_{0,3} = 0.025 \text{ [lu]}$$

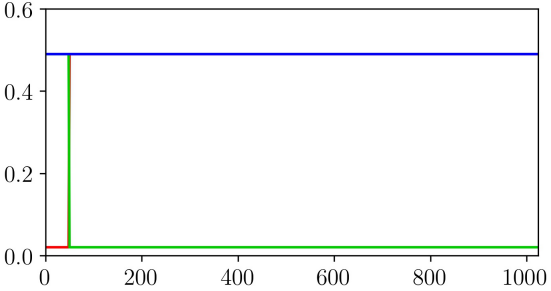
Diffusion coefficients

$$\mathcal{D}_{mn} = 10^{-3} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \text{ [lu]}$$

Viscous fingering

3 species - stable initial configuration, viscous fingering





3 species → RGB channels

$$x_1 = 0.02\ R \quad x_2 = 0.49\ G \quad x_3 = 0.49\ B$$

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Pure viscosity

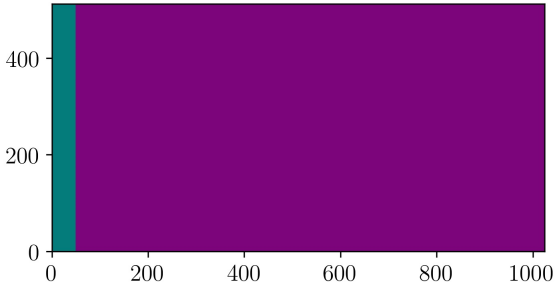
$$\mu_{0,1} = 0.5 \text{ [lu]}$$
$$\mu_{0,2} = 0.5 \text{ [lu]}$$
$$\mu_{0,3} = 0.025 \text{ [lu]}$$

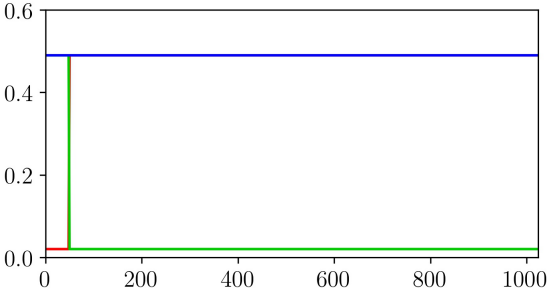
Diffusion coefficients

$$\mathcal{D}_{mn} = 10^{-3} \begin{pmatrix} 0 & 1 & 10 \\ 1 & 0 & 0.1 \\ 10 & 0.1 & 0 \end{pmatrix} \text{ [lu]}$$

Viscous fingering

3 species - stable initial configuration, viscous fingering





Causes

- multicomponent effects: osmotic & reverse diffusion
- result in a localised less viscous slice of fluid

Consequences

- viscous fingering in spite of an initial stable configuration
- fingers mostly composed of the third species

Conclusion

Method

- We propose a LB model for multi-species flow using an inter-molecular friction force.
- Both gray lattice Boltzmann and Brinkman forcing schemes leads to identical results in this case.

✓ **Simulation of miscible viscous fingering instability by the LBM** ✓

Physics

- Mixing length: 2 regimes are identified (diffusive then advective).
- High Péclet numbers result in a more intense instability.
- **3 species**: an initial stable configuration may become unstable because of multi-component effects (preliminary result).

Current and future work

- Detailed comparison against a linear stability analysis in the case of two species.
- Investigation of three species viscous fingering.
- Pore-scale simulation of the viscous fingering instability.

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Thank you for your attention.

Any questions?

Macroscopic equations

Chapman and Enskog expansion procedure

$$\partial_t \rho_m + \nabla \cdot (\rho_m \mathbf{u}_m) = 0$$

$$\partial_t(\rho_m \mathbf{u}_m) + \nabla \cdot (\rho_m \mathbf{u}_m \otimes \mathbf{u}_m) = -\nabla p_m + \nabla \cdot \left[\mu_m \left(\nabla \mathbf{u}_m + (\nabla \mathbf{u}_m)^T\right)\right] - p \sum_{n=1}^{N} \frac{x_m x_n}{\mathcal{D}_{mn}} (\mathbf{u}_m - \mathbf{u}_n) + \mathcal{F}_{B,m}$$

$$p_m = \rho_m c_s^2, \quad p = \sum_{m=1}^{N} p_m$$

$$\mu_m = \rho_m c_s^2 (\tau_m - \frac{\delta_t}{2})$$

Modifying the speed of sound using a body force

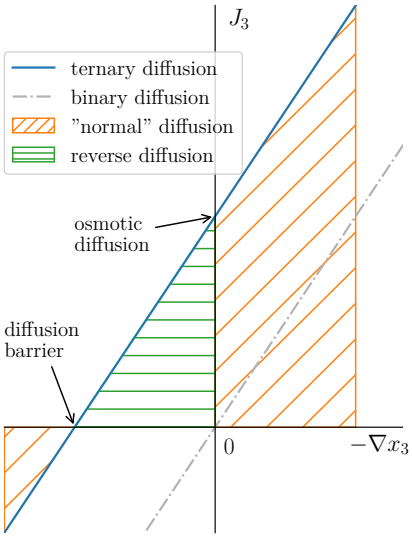
Buick et al. 2006

$$\mathcal{F}_{B,m} = (1 - \beta_m) c_s^2 \nabla \rho_m$$

gradient term is computed adopting a compact scheme

$$\nabla \rho_m(\mathbf{x}) = \frac{1}{c_s^2} \sum_{\alpha} \omega_\alpha \mathbf{e}_\alpha \rho_m(\mathbf{x} + \mathbf{e}_\alpha)$$

and the species equation of state is then equal to

$$p_m = \beta_m c_s^2 \rho_m = c_{s,m}^2 \rho_m$$

Multi-component effects