Simulation of multi-component flows by the lattice Boltzmann method and application to the viscous fingering instability

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Examiners: P. Sagaut & F. Dubois

PhD defense – December 3rd, 2019
Mass transfer is ubiquitous in natural phenomena and industrial applications.

- Oceanic (thermohaline) circulation
- Combustion, energy production, rocket propulsion
- Chemistry, food processing, pharmacy, biology
- Microfluidics, lab on a chip (image published by The Royal Society of Chemistry)

Mixing in tight space and porous medium:
- Difficult (molecular diffusion)
- Mixing with dissimilar viscosities ↔ viscous fingering instability
Context

Transport phenomena

- transport of momentum
- transport of energy
- transport of mass of various chemical species

From a molecular point of view, all these mechanisms are related to the collision of molecules.

→ Kinetic theory and Lattice Boltzmann method are based on a statistical description and provide a unified way to deal with transport phenomena.
Simulation of multi-component flows by the lattice Boltzmann method and application to the viscous fingering instability

Introduction
  Kinetic theory of gas
  Lattice Boltzmann method (LBM)

Multi-component flows using LBM
  Proposed model
  Numerical validation

Viscous fingering instability using LBM
  Porous medium model
  Viscous fingering: binary mixture
  Viscous fingering: ternary mixture
Introduction

Kinetic theory of gas

Fluid $\iff$ molecules moving around and colliding

- Position $\mathbf{x} = (x, y, z)$
- Velocity $\mathbf{e} = (e_x, e_y, e_z)$
- Time $t$
Introduction

Kinetic theory of gas

Fluid \(\iff\) molecules moving around and colliding

- Position \(\mathbf{x} = (x, y, z)\)
- Velocity \(\mathbf{e} = (e_x, e_y, e_z)\)
- Time \(t\)

Statistical description

\(f(x, e, t)\): distribution function

\(\rightarrow\) density of molecules with a velocity \(e\) at position \(x\) and time \(t\).

Boltzmann equation:

\[
\frac{\partial f}{\partial t} + \mathbf{e} \cdot \nabla f + \frac{F_B}{\rho} \cdot \nabla_e f = \left( \frac{df}{dt} \right)_{\text{coll}}
\]
Introduction

Kinetic theory of gas

Fluid $\Leftrightarrow$ molecules moving around and colliding

$\uparrow$ Position $x = (x, y, z)$  $\uparrow$ Velocity $e = (e_x, e_y, e_z)$  $\uparrow$ Time $t$

Statistical description

$f(x, e, t)$: distribution function
$\rightarrow$ density of molecules with a velocity $e$ at position $x$ and time $t$.
Boltzmann equation:

$$\frac{\partial f}{\partial t} + e \cdot \nabla f + \frac{F_B}{\rho} \cdot \nabla_e f = \left( \frac{df}{dt} \right)_{coll}$$

Macroscopic moments

$\uparrow$ $\rho(x, t) = \int f(x, e, t)de,$
$\uparrow$ $\rho(x, t)u(x, t) = \int ef(x, e, t)de,$
$\uparrow$ $\rho(x, t)E(x, t) = \int \frac{1}{2}e^2 f(x, e, t)de.$
Introduction

Kinetic theory of gas

Fluid \leftrightarrow \text{molecules moving around and colliding}

\begin{itemize}
  \item Position \( x = (x, y, z) \)
  \item Velocity \( e = (e_x, e_y, e_z) \)
  \item Time \( t \)
\end{itemize}

Statistical description

\( f(x, e, t) \): distribution function

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Macroscopic moments

\begin{itemize}
  \item \( \rho(x, t) = \int f(x, e, t) \, de \),
  \item \( \rho(x, t) u(x, t) = \int e f(x, e, t) \, de \),
  \item \( \rho(x, t) E(x, t) = \int \frac{1}{2} e^2 f(x, e, t) \, de \).
\end{itemize}
1. Bhatnagar-Gross-Krook (BGK) collision operator

\[ \frac{df}{dt}_{\text{coll}} = -\frac{1}{\tau} (f - f^{eq}) \]

with \( f^{eq}(x, e, t) \) Maxwell-Boltzmann distribution (Gaussian-like).

- Capture the relaxation of \( f \) toward an equilibrium state according to the relaxation time \( \tau \).
- Chapman-Enskog expansion shows that Navier-Stokes equations are recovered, and
- \( \tau \) is related to the fluid viscosity.

Note: Other more advanced relaxation operators exist to remedy some numerical stability defects.
2. Velocity space discretization

- Macroscopic moments conservation ($\int \cdot d\mathbf{e} = \sum_{\alpha}$ up to a certain order)
- Only a few velocities are required to recover the macroscopic behavior of the fluid (mass and momentum transport)

\[
\frac{\partial f_\alpha}{\partial t} + \mathbf{e}_\alpha \cdot \nabla f_\alpha = -\frac{1}{\tau} (f_\alpha - f_{eq}^\alpha) + S_\alpha
\]

\[\alpha = 1, \ldots, 9\]

\[f_\alpha = \begin{pmatrix} f_1 \\ \vdots \\ f_9 \end{pmatrix}\]

\[\rho = \sum_\alpha f_\alpha\]

\[f_{eq}^\alpha = \rho \omega_\alpha \left[1 + \frac{\mathbf{u} \cdot \mathbf{e}_\alpha}{c_s^2} + \frac{(\mathbf{u} \cdot \mathbf{e}_\alpha)^2}{2c_s^4} - \frac{\mathbf{u} \cdot \mathbf{u}}{2c_s^2}\right]\]

\[\rho \mathbf{u} = \sum_\alpha \mathbf{e}_\alpha f_\alpha\]

\[S_\alpha = \omega_\alpha \left[\frac{\mathbf{e}_\alpha \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_\alpha \cdot \mathbf{u}) \mathbf{e}_\alpha}{c_s^4}\right] \cdot \mathbf{F}_B\]
3. Physical space and time discretization

Integration along the characteristics $e_{\alpha}$: space, time, and kinetic velocities $e_{\alpha}$ coupling.

$$f_\alpha(x + e_\alpha \delta t, t + \delta t) = f_\alpha(x, t) - \frac{\delta t}{\tau} [f_\alpha(x, t) - f^{eq}_\alpha(x, t)] + \delta t (1 - \frac{\delta t}{2\tau}) S_\alpha$$

$$\rho = \sum_\alpha f_\alpha$$

$$f^{eq}_\alpha = \rho \omega_\alpha \left[ 1 + \frac{u \cdot e_\alpha}{c_s^2} + \frac{(u \cdot e_\alpha)^2}{2c_s^4} - \frac{u \cdot u}{2c_s^2} \right]$$

$$\rho u = \sum_\alpha e_\alpha f_\alpha + \frac{1}{2} F_B$$

$$S_\alpha = \omega_\alpha \left[ \frac{e_\alpha - u}{c_s^2} + \frac{(e_\alpha \cdot u)e_\alpha}{c_s^4} \right] \cdot F_B$$
Introduction

Lattice Boltzmann method - LBM algorithm

\[ f_\alpha(x + e_\alpha \delta t, t + \delta t) = f_\alpha(x, t) - \frac{\delta t}{\tau} [f_\alpha(x, t) - f_{eq\alpha}(x, t)] + \delta t (1 - \frac{\delta t}{2\tau}) S_\alpha \]
Introduction

Lattice Boltzmann method - LBM algorithm

\[ f_\alpha(x + e_\alpha \delta_t, t + \delta_t) = f_\alpha(x, t) - \frac{\delta_t}{\tau} [f_\alpha(x, t) - f_{\alpha eq}(x, t)] + \delta_t (1 - \frac{\delta_t}{2\tau}) S_\alpha \]

Collide and Stream algorithm

```
init
```

\[ f_\alpha(x, t = 0) = f_{\alpha eq}(\rho(x, 0), u(x, 0)) \]
Introduction

Lattice Boltzmann method - LBM algorithm

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→ Collide and Stream algorithm

init → collide
Introduction

Lattice Boltzmann method - LBM algorithm

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f_\alpha(x + e_\alpha \delta_t, t + \delta_t) = f_\alpha(x, t) - \frac{\delta_t}{\tau} [f_\alpha(x, t) - f^{eq}_\alpha(x, t)] + \delta_t (1 - \frac{\delta_t}{2\tau}) S_\alpha
\]

Collide and Stream algorithm

- **init**
- **collide**

stream
Introduction

Lattice Boltzmann method - LBM algorithm

\[ f_\alpha(x + e_\alpha \delta t, t + \delta t) = f_\alpha(x, t) - \frac{\delta t}{\tau} [f_\alpha(x, t) - f_\alpha^{eq}(x, t)] + \delta t (1 - \frac{\delta t}{2\tau}) S_\alpha \]

Collide and Stream algorithm

\[ \rightarrow \text{Collide and Stream algorithm} \]

init \rightarrow collide \rightarrow stream \rightarrow apply \ BCs
Introduction

Lattice Boltzmann method - LBM algorithm

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f_{\alpha}(x + e_{\alpha} \delta_t, t + \delta_t) = f_{\alpha}(x, t) - \frac{\delta_t}{\tau} \left[ f_{\alpha}(x, t) - f_{\alpha}^{eq}(x, t) \right] + \delta_t \left( 1 - \frac{\delta_t}{2\tau} \right) S_{\alpha}
\]

Collide and Stream algorithm

init \rightarrow collide \rightarrow stream \rightarrow compute moments \rightarrow apply BCs

\[
\rho = \sum_{\alpha} f_{\alpha}
\]

\[
\rho u = \sum_{\alpha} e_{\alpha} f_{\alpha} + \frac{1}{2} F_B
\]
Introduction

Lattice Boltzmann method - LBM algorithm

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→ Collide and Stream algorithm

Advantages

▶ simple yet physically based on the Boltzmann equation
▶ 2nd order accurate for the weakly compressible NS equations
▶ efficient and HPC ready (parallel architectures and GPU)

Limitations

▶ uniform grid
▶ low Mach number flow (< 0.3)
▶ isothermal flow
Introduction

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Multi-component flows using LBM

- Proposed model
- Numerical validation

Viscous fingering instability using LBM

- Porous medium model
- Viscous fingering: binary mixture
- Viscous fingering: ternary mixture
Multi-species using LBM

Species distribution functions

\[ f^m_\alpha (x, t) \]

→ Each species \( m \) has its own distribution function which is governed by its own kinetic equation.

\[ \rho_m = \sum_\alpha f^m_\alpha, \]
\[ \rho_m u_m = \sum_\alpha f^m_\alpha e_\alpha \]

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

Limitations: mixture-averaged transport coefficient, free parameters, collision is greatly modified.
Multi-species using LBM

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Limitations: mixture-averaged transport coefficient, free parameters, collision is greatly modified.

Solution

→ Diffusion interaction among species is taken into account by means of a force.
→ Since collision is not altered, this method can easily be introduced in any existing LB algorithm.
Multi-species using LBM

Part 1: viscous species dissipation

\[ f^m_{\alpha}(x + e_\alpha \delta_t, t + \delta_t) = f^m_{\alpha}(x, t) - \frac{\delta_t}{\tau_m} \left[ f^m_{\alpha}(x, t) - f^{m(eq)}_{\alpha}(x, t) \right] \]

\[ \rightarrow \] Each species \( m \) has its own distribution function which is governed by its own kinetic equation.

\[ \rho_m = \sum_\alpha f^m_{\alpha}, \]
\[ \rho_m u_m = \sum_\alpha f^m_{\alpha} e_\alpha \]

\[ f^{m(eq)}_{\alpha} = \rho_m \omega_\alpha \left[ 1 + \frac{u_m \cdot e_\alpha}{c_s^2} + \frac{(u_m \cdot e_\alpha)^2}{2c_s^4} - \frac{u_m \cdot u_m}{2c_s^2} \right] \]

How to choose the relaxation time \( \tau_m \)?

\[ \rightarrow \] From the kinetic theory of gases!

Hirschfelder, Curtiss, and Bird 1954; Kerkhof and Geboers 2004

\[ \mu_m = \frac{x_m \mu_{0,m}}{\sum_N x_n \Phi_{mn}}, \quad \mu_m = \rho_m c_s^2 (\tau_m - \frac{\delta_t}{2}) \]
Multi-species using LBM

Part 2: molecular species diffusion

\[ f^m_\alpha (x + e_\alpha \delta_t, t + \delta_t) = f^m_\alpha (x, t) - \frac{\delta_t}{\tau_m} \left[ f^m_\alpha (x, t) - f^{m(eq)}_\alpha (x, t) \right] + \delta_t (1 - \frac{\delta_t}{2\tau_m}) S^m_\alpha (x, t) \]

→ Each species \( m \) has its own distribution function which is governed by its own kinetic equation.

\[ \rho_m = \sum_\alpha f^m_\alpha, \]
\[ \rho_m u_m = \sum_\alpha f^m_\alpha e_\alpha + \frac{1}{2} F_{D,m} \]

\[ f^{m(eq)}_\alpha = \rho_m \omega_\alpha \left[ 1 + \frac{u_m \cdot e_\alpha}{c_s^2} + \frac{(u_m \cdot e_\alpha)^2}{2c_s^4} - \frac{u_m \cdot u_m}{2c_s^2} \right] \]
\[ S^m_\alpha = \omega_\alpha \left[ \frac{e_\alpha - u_m}{c_s^2} + \frac{(e_\alpha \cdot u_m) e_\alpha}{c_s^4} \right] \cdot F_{D,m} \]

Inter-molecular friction force

\[ F_{D,m} = -p \sum_{n=1}^{N} \frac{x_m x_n}{D_{mn}} (u_m - u_n) \]

\( D_{mn} \): Maxwell-Stefan diffusion coefficient

Maxwell 1867; Chapman and Cowling 1932; Hirschfelder, Curtiss, and Bird 1954; Kerkhof and Geboers 2004
Multi-species using LBM

Numerical validation

Numerical validation

- A-Decay of a density wave (↔ molar mass ratio up to 86)
- B-Equimolar counter-diffusion
- C-Loschmidt’s tube
- D-Opposed jets flow
Multi-species using LBM
C-Loschmidt’s tube

Loschmidt’s experiment: a ternary mixture exhibiting complex diffusion.

\[ x_{Ar} = 0.509 - \delta \]
\[ x_{CH_4} = 0 + 2\delta \]
\[ x_{H_2} = 0.491 - \delta \]
\[ x_{Ar} = 0.485 - \delta \]
\[ x_{CH_4} = 0.515 - \delta \]
\[ x_{H_2} = 0 + 2\delta \]

Sketch of the experimental apparatus. \( \delta = 5 \times 10^{-4} \).

\[
\begin{array}{c|c|c|c}
L_{\text{ref}} & [m] & 2\pi \sqrt{1/60} \\
p & [\text{Pa}] & 101325 \\
T & [\text{K}] & 307.15 \\
\hline
m & Ar & CH_4 & H_2 \\
\hline
M_m & [g/mol] & 39.948 & 16.0425 & 2.01588 \\
D_{Ar_m} & [\text{mm}^2/\text{s}] & - & 21.57 & 83.35 \\
D_{CH_4 m} & [\text{mm}^2/\text{s}] & 21.57 & - & 77.16 \\
D_{H_2 m} & [\text{mm}^2/\text{s}] & 83.35 & 77.16 & - \\
\mu_{0,m} & [\mu\text{Pa/s}] & 22.83 & 11.35 & 9.18 \\
\end{array}
\]

Physical parameters of the experiment.

The left and right mean compositions are measured in time during the mixing.
Multi-species using LBM

C-Loschmidt’s tube

\[ t^* = t \times \frac{D_{\text{ArCH}_4}}{L_{\text{ref}}^2} \]

- (lines) simulation;
- (symbols) experimental data extracted from Krishna 2015

Molar fraction vs. scaled time for different species.
Multi-species using LBM

C-Loschmidt’s tube

Diffusion of Argon

- $t^* < 0.04$
  - left $\leftarrow$ right tubes

- $0.04 < t^* < 0.05$
  - left $\leftrightarrow$ right tubes

- $t^* > 0.05$
  - left $\rightarrow$ right tubes

Is something wrong?

$D_{ArH_2} = 83.35 \text{ mm}^2/\text{s}$

$D_{ArCH_4} = 21.57 \text{ mm}^2/\text{s}$

$J_m = \frac{t^*}{D_{ArCH_4}/L_{ref}^2}$

(lines) simulation ;

(symbols) experimental data extracted from Krishna 2015

Multi-component diffusion effects
Multi-species using LBM

Two opposed jets of a quaternary mixtures: a convection-diffusion competing mechanism.

Molar fraction and velocity streamline plot of $H_2O$.

- (lines) present method;
- (symbols) LBM from Arcidiacono et al. 2007 at $y = n_y/2$. 

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PhD defense – 16 of 34
Multi-species using LBM

Synthesis

- Each species has its own distribution function which is governed by its own kinetic equation.
- Viscous dissipation is related to the relaxation toward the equilibrium.
- Molecular diffusion is associated with the inter-molecular diffusion force.
- Transport coefficients are calculated from the kinetic theory of gases.
- Species with dissimilar molecular masses are simulated by using an artificial force.

- Multi-component diffusion effects are recovered.
- The simple structure of the collide and stream algorithm is preserved.
- Proposed model is independent of the collision operator.
- Only a few modifications are needed to upgrade an existing single-fluid code to take into account diffusion between multiple species.
Introduction
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Multi-component flows using LBM
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Viscous fingering instability using LBM
  - Porous medium model
  - Viscous fingering: binary mixture
  - Viscous fingering: ternary mixture
Viscous fingering

This instability occurs when a less viscous fluid displaces a more viscous fluid in a porous medium. Improve the mixing efficiency in porous media or be detrimental in

- oil recovery
- CO₂ sequestration

→ Nijjer et al. 2018 after a shutdown time of 150 years: mixing zone of 50km long with fingering / 5m long with only pure diffusion

- chromatography column
- soil contamination

Viscous fingering in a Hele-Shaw cell. 
_Homsy 1987_

Viscous fingering in an opaque medium visualized by X-ray absorption.
Viscous fingering using LBM

Core ingredients of the instability

Viscous fingering a complex convection-diffusion mechanism.
We need a

- binary miscible flow → inter-molecular friction force
- with a disparity in viscosity → partial viscosities
- in a porous medium → ?

Porous medium

Explicit: model the pores of the porous medium (computationally expensive)

Implicit: use a model

- Average view of the porous medium: permeability $K$
- Less computationally expensive
- Comparison with the literature (Darcy’s law)
Gray lattice Boltzmann (GLBM)

Porous medium effect $\sim$ partial bounce-back.

*Yoshida and Hayashi 2014*: Post-collision distribution functions are reflected.

$\theta_m = 0 \Rightarrow$ standard streaming

$\theta_m = 1 \Rightarrow$ bounce-back condition

$\theta$ is the amount of reflection

$\theta_m = 0 \Rightarrow$ standard streaming

$\theta_m = 1 \Rightarrow$ bounce-back condition

Brinkman forcing scheme (BF)

Porous medium effect $\sim$ global drag effect.

*Martys 2001, Guo and Zhao 2002, Ginzburg 2008*

$$F_{\text{porous},m} = -\frac{\mu_m}{K} \mathbf{u}_m$$

$$\frac{2\theta_m}{(1 - \theta_m)\delta_t} = \frac{\mu_m}{K\rho_m}$$
Viscous fingering using LBM

Numerical configuration

Initial conditions
\[ f^m_\alpha(t = 0) = f^{m(eq)}_\alpha(\rho_m, u_{x,m} = U, u_{y,m} = 0) \]

Grid resolution
Resolution corresponding to
- \( n_y = 4000 \) to study the early times
- \( n_y = 2000 \) to study the intermediate times

Dimensionless numbers
\[ R = \ln \left( \frac{\mu_{0,2}}{\mu_{0,1}} \right) = 3 \]
\[ Pe = \frac{UL_{\text{ref}}}{D_{12}} = [500...5000] \]
\[ Re_{0,1} = \frac{\rho_{\text{ref}}UL_{\text{ref}}}{\mu_{0,1}} = 10 \]
\[ Da = \frac{K}{L^2_{\text{ref}}} = 6.25 \times 10^{-8} \]
\[ Ma = \frac{U}{c_s} = \sqrt{3} \times 10^{-3} \]
Viscous fingering using LBM
Global dynamics

BF scheme, Pe=2000.

Fingers development
▶ Coarsening of the fingers in the transverse direction.
▶ Growth of the fingers in the streamwise direction

Early times: linear interactions
▶ Initial planar interface starts to deform
▶ Small fingers develop

Intermediate times: non-linear interactions
▶ spreading, shielding, fading, coalescence
▶ tip splitting, and side branching
Viscous fingering using LBM

Intermediate times: mixing length

Mixing length

\[ l_{mix}(t) = \| \bar{X}_{x_1=0.89}(t) - \bar{X}_{x_1=0.11}(t) \| \]

\[ t^* = tU/L_{ref} \]
Viscous fingering using LBM

Intermediate times: mixing length

- **Diffusion-dominated regime** \( l_{\text{mix}} \sim \sqrt{t^*} \)
- **Advection-dominated regime** \( l_{\text{mix}} \sim t^* \)
- **No difference between GLBM and BF schemes**
Viscous fingering using LBM

Early times: perturbation

Assuming a perturbation

\[ x'_m(x, t) = x'_m(x) \exp(\sigma t) \]

Growth rate of the perturbation \( \sigma \)

\[ x'_m(x, t) = x^0_m(x, t) - x_m(x, t) \]

\[ \hat{x}(x, k, t) = \text{FFT}_y (x'_m(x, t)) \]

\[ a(k, t) = \|\hat{x}(x, k, t)\|_2 = \sqrt{\int \hat{x} \cdot \hat{x}^\dagger \, dx} \]

\[ \sigma(k, t) = \frac{d \ln(a(k, t))}{dt} \]

\( x^0_m \): base state \( \iff \) non-perturbed simulation.
Viscous fingering using LBM

Early times: influence of the porous model

Dispersion curve for Pe = 2000 at various times from $t^* = 0.005$ to $t^* = 0.1$ with a time step $\Delta t^* = 0.05$.

- 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 using LBM

Early times: influence of the Péclet number $Pe = \frac{UL_{\text{ref}}}{D_{12}}$

▶ High Péclet numbers lead to a more intense instability.
▶ The range of unstable wave numbers and the growth rate increase with $Pe$.
▶ The Péclet number influences the transition from linear to non-linear interactions.
Viscous fingering using LBM

Early times: influence of the Péclet number $\text{Pe} = \frac{UL_{\text{ref}}}{D_{12}}$

- Symbols: linear stability analysis with quasi-steady-state approximation (QSSA).
- QSSA is known to have some flaws for very short times (compared to IVP, non-modal analysis) Hota et al. 2015.
- Excellent agreement for $t^* = 0.1$.

$\sigma^t = 0.01$:

- $\text{Pe} = 5000$
- $\text{Pe} = 2000$
- $\text{Pe} = 1000$
- $\text{Pe} = 500$

$\sigma^t = 0.1$:

- $\text{Pe} = 5000$
- $\text{Pe} = 2000$
- $\text{Pe} = 1000$
- $\text{Pe} = 500$
Viscous fingering using LBM
from binary to ternary mixture

What are the differences between two and three species?

<table>
<thead>
<tr>
<th>Binary mixture</th>
<th>Ternary mixture</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_{12} = D_{21}$</td>
<td>$D_{12} \neq D_{13} \neq D_{23}$</td>
</tr>
<tr>
<td>$x_1 = 1 - x_2$</td>
<td>$x_1 + x_2 + x_3 = 1$</td>
</tr>
<tr>
<td>$\nabla x_1 = -\nabla x_2$</td>
<td>$\nabla x_1 + \nabla x_2 + \nabla x_3 = 0$</td>
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$\leftrightarrow$ Multi-component diffusion effects
Viscous fingering using LBM

ternary mixtures: fingering induced by reverse diffusion

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<th>Displaced fluid</th>
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<td>$x_1$ (R)</td>
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</tr>
<tr>
<td>$x_3$ (B)</td>
<td>0.45</td>
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RGB color

- R: Red
- G: Green
- B: Blue

Pe = 5000

$Re_{0,1} = 10$

$R_{12} = \ln\left(\frac{\mu_{0,1}}{\mu_{0,2}}\right) = 0$

$R_{13} = \ln\left(\frac{\mu_{0,1}}{\mu_{0,3}}\right) = 3$

$D_{mn} = \frac{L_{ref} U}{Pe} \begin{pmatrix} 0 & 1 & 0.1 \\ 1 & 0 & 1 \\ 0.1 & 1 & 0 \end{pmatrix}$
Viscous fingering using LBM

ternary mixtures: fingering induced by reverse diffusion

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$R_{12} = \ln\left(\frac{\mu_{0,1}}{\mu_{0,2}}\right) = 0$

$R_{13} = \ln\left(\frac{\mu_{0,1}}{\mu_{0,3}}\right) = 3$

$D_{mn} = \frac{L_{ref} U}{Pe} \begin{pmatrix} 0 & 1 & 0.1 \\ 1 & 0 & 1 \\ 0.1 & 1 & 0 \end{pmatrix}$

![Image of fingering pattern]
Viscous fingering using LBM

ternary mixtures: fingering induced by reverse diffusion

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
Viscous fingering using LBM
ternary mixtures: fingering induced by reverse diffusion

Species fingering

- Third species: interface significantly deformed. Reverse diffusion tends to accentuate the fingering.
- Second species: $D_{12} = D_{23} \leftrightarrow$ almost symmetric interface.
- First species: $D_{13} < D_{12} \leftrightarrow$ fingers of low concentration are dragged along the third species.

Color-map of the molar fraction at $t^* = 1.8$ for each species
The physics of the binary viscous fingering instability is recovered for early times (growth rates) for intermediate times (diffusive then advective regimes).

Both BF and GLBM schemes lead to equivalent results for the observed case.

Behavior of the instability can dramatically change for three and more species.

Viscous fingering could be induced by reverse diffusion despite having an initial stable flow configuration.
Conclusion

- A lattice Boltzmann method for multi-component flows is proposed.
- Standard relaxation process $\rightarrow$ viscous dissipation (partial viscosities).
- Inter-molecular-friction force $\rightarrow$ molecular diffusion (Maxwell-Stefan diffusion coefficient).
- Basic features of the model are validated.
- The physics of the binary viscous fingering instability is recovered.
- The influence of reverse diffusion on the instability is highlighted.
Perspectives

- Further studies are required on the multi-component model
- Parametric study of the ternary viscous fingering (passive control of viscous fingering).
- Explicit model of the porous medium

- 3D simulations

- Gravity currents and double-diffusive convection problems in oceans
Thank you for your attention.

Any questions?
Why not an advection-diffusion equation?

Diffusion equation is postulated, and a kinetic scheme is tailored to solve it.

\[ \partial_t c_m + \nabla \cdot (c_m u) = -J_m \]

\[ J_1 = -c_t D_{11} \nabla x_1 - c_t D_{12} \nabla x_2 \]
\[ J_2 = -c_t D_{21} \nabla x_1 - c_t D_{22} \nabla x_2 \]
\[ \text{and } J_3 = -J_1 - J_2 \]

Generalized Fick’s law (ternary mixture)

Not as practical as the Maxwell-Stefan approach \( (\nabla x_m = \sum_{n=1}^{N} \frac{x_m J_n - x_n J_m}{c_t D_{mn}}) \) to mass transfer

- 4 Fick diffusion coefficients for a ternary mixture.
- \( D \) may be positive, negative, are usually non-symmetric and vary according to the mixture composition.
- \( D_{mn} \) do not reflect the \( m - n \) interaction (collision). Its value depends on the component numbering.
Power spectral density at different times $t^*$ for different resolutions equivalent to blue, $n_y = 4000$; orange, $n_y = 2000$; green, $n_y = 1000$. $G = \hat{x}\hat{x}^\dagger$ where $\hat{x}^\dagger$ is the conjugate of the Fourier coefficients $\hat{x}$. $G$ is normalized by its variance: $\sigma(G)$. 

\[ t^* = 0.03125, \quad t^* = 0.125, \quad t^* = 0.375 \]
Convergence study

Contour-plots and mixing length

Contour plot for $x_1 = 0.4$ at $t^* = 0.125$ and $t^* = 0.375$. 

Mixing length according to $t^*$. 

- $n_y = 4000$
- $n_y = 2000$
- $n_y = 1000$