

#### NAZARBAYEV UNIVERSITY

Multiphase flow in a porous medium using Lattice Boltzmann Method and grid verification

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#### **Related Publications**

- Ashirbekov, A., Kabdenova, B., Monaco, E., & Rojas-Solórzano, L. R. (2021). Equation of State's Crossover Enhancement of Pseudopotential Lattice Boltzmann Modeling of CO2 Flow in Homogeneous Porous Media. *Fluids*, 6(12), 434.
- In Progress
  - Numerical Study of the Effect of Viscosity Ratio on the CO2 Injection Through a Homogeneous Aquifer Using a Crossover-EoS Pseudopotential Lattice Boltzmann Model



## Outline

- 1. Motivation
- 2. Aims and objectives
- 3. Lattice Boltzmann Method, its principles and governing equations
- 4. Method for grid verification
- 5. Validation of formulation
- 6. Domain verification; Results of multiphase analysis
- 7. Conclusion



# Motivation

- Fluid flows with multiscale and multiphase phenomena
- Energy systems: power plants, fuel cells, generators, turbines
- Medicine: blood flow
- Geoscience: CO2 sequestration, oil recovery



(Cordero et al., 2018)



# Motivation: CO<sub>2</sub> sequestration

- Long-term storage of excess carbon dioxide captured from the atmosphere
- One of the key strategies for reducing CO2 emission rates
- The global emission of CO2 alone can rise by 6.41 billion tonnes, 18% of 2021, by 2030 by estimations of EIA



Injection of CO<sub>2</sub> into the porous medium of water saturated oil



### Motivation: CO<sub>2</sub> sequestration modeling

- CO<sub>2</sub> sequestration involves modeling of porous medium, which is small scale and multiphase
- Is analyzed using different approaches and methods
- Lattice Boltzmann method was tried, however only with color-fluid model, and without discretization verification
- Hypothesis: pseudopotential LBM modeling, verified with domain size analysis, can give useful insight into mechanics of CO<sub>2</sub> sequestration



### Aims and objectives

- Main goal: model the immiscible displacement flow in a porous medium and apply grid verification
  - 1. Introducing the multi-component LBM formulation
  - 2. To develop validation static case to confirm formulation stability
  - 3. To develop and perform domain size verification procedure



#### Lattice Boltzmann Method

- Finite volume, the volume of fluid, and level-set methods most used models, traditional FVM CFD
- Those methods are macroscopic, with assumption of fluid as a continuum

- Lattice Boltzmann Method (LBM) mesoscale method
- Assumes fluid as a collection of particles





# LBM Principles

- Particle interactions but focus on macroscopic behavior
- Fluid is treated as a collection of discrete particles on a uniform grid
- Based on microscopic models and kinetic theory
- Deals with interactions of particles



LBM lattice, probability function and directions, 2D case ("Lattice Boltzmann Method", 2021)



## Governing equations

$$f_i^{\ j}(\mathbf{x} + \mathbf{e_i}\Delta t, t + \Delta t) - f_i^{\ j}(\mathbf{x}, t) = -\frac{1}{\tau^j} \Big( f_i^{\ j}(\mathbf{x}, t) - f_i^{\ j, eq}(\mathbf{x}, t) \Big)$$

streaming (LHS) and collision (RHS) steps of distribution function, derived from Boltzmann equation

$$f_i^{j,eq}(\mathbf{x},t) = \omega_i \rho^j \left[ 1 + \frac{\mathbf{e_i} \cdot \mathbf{u^j}}{c_s^2} + \frac{\left(\mathbf{e_i} \cdot \mathbf{u^j}\right)^2}{2c_s^4} - \frac{\left(\mathbf{u^j}\right)^2}{2c_s^2} \right]$$

Maxwell-Boltzmann equilibrium

 $\rho^{j} \mathbf{u}^{j} = \sum_{i} f_{i}^{j} \mathbf{e}_{i}$  momentum – relation to physical density



# Governing equations (cont.)

$$\mathbf{F}_{int}{}^{j}(\mathbf{x},t) = -G(\mathbf{x},\mathbf{\dot{x}}) \rho^{j}(\mathbf{x},t) \sum_{i} \omega_{i} \psi^{j}(\mathbf{x}+\mathbf{e}_{i}\Delta t,t) \mathbf{e}_{i} \quad \text{interaction between components}$$

$$\mathbf{F}_{wet}{}^{j}(\mathbf{x},t) = -g_{wall}{}^{j}\rho^{j}(\mathbf{x},t) \sum_{i} \omega_{i}s(\mathbf{x}+\mathbf{e}_{i})\mathbf{e}_{i} \quad \text{interaction with obstacles}$$

$$\mathbf{u}_{eq}{}^{j} = \mathbf{u}^{j} + \frac{\tau^{j}}{\rho^{j}}(\mathbf{F}_{int} + \mathbf{F}_{wet})^{j}\Delta t \quad \text{forces effect transferring to distribution function}$$

 $\psi^{j}(\mathbf{x},t) = \rho_{0} - exp(-\rho(\mathbf{x},t)/\rho_{0})$  pseudopotential

$$v = c_s^2 \sum_j \chi^j (\tau^j - 0.5)$$
 kinetic viscosity



## Grid verification

- Lack of studies to perform the proper domain verification
- In 3D typically done by increasing number of directions (D3Q15  $\rightarrow$  D3Q27)
- Not commonly applied in 2D, and is not trivial with lack of software capabilities



#### Grid verification – issues



Simple increase in domain size

Coordinate scaling



# Grid verification – proposed solution

- Conversion of the domain into pixelated image, each lattice point is one pixel
- Color and opacity may be used to decode state of lattice point (e.g. components, initial velocities)
- Perform scaling using image scaling techniques





Domain converted to image



### Grid verification – proposed solution



Scaling using image processing, nearest neighbor scaling



### Grid verification



Original

Coordinate scaling

Proposed solution



#### Validation – droplet test



201×201 lattice unites

$$g = 1$$

$$\rho_{water} = 4.3, \, \rho_{CO2} = 1$$

 $\tau_{water} = \tau_{CO2} = 1$ 



Density profile (in LU) at the crosssection of the domain taken at the horizontal



Water in red,  $CO_2$  is in blue

#### Validation – contact angle, wettability

$\theta_{eq}$	$g_{CO_2,wall}$	$g_{H_2O,wall}$		
70°	0.2	-0.2		
90°	0	0		
120°	-0.2	0.2		
130°	-0.3	0.3		





## Porous medium model



0 ts



Water in blue,  $CO_2$  in red,  $\theta_{eq} = 70^{\circ}$  viscosity ratio of 1



4800 ts

7100 ts



#### Domain size verification



Line probe location (shown in black) in the gridindependence analysis of  $CO_2$  penetration LBM model



#### Domain size verification

Velocity over line probe

• 401x201 • 601x301 • 801x401



Grid size, LU <sup>2</sup>	$CO_2$ flux, ×10^-7 LU/ts	Relative error (%)
401×201	3.590	-
601×301	3.651	1.7%
801×401	3.679	0.76%

Time-space average  $\text{CO}_2$  flux over a probe line integrated over 7100 timesteps

Average velocity magnitude along the probe line versus timesteps



### CO<sub>2</sub> sequestration conditions

Temperature (K)	308	318	328	338
Water viscosity (Pa · s)	$7.4 \times 10^{-4}$	$6.1 \times 10^{-4}$	$5.2 \times 10^{-4}$	$4.4  imes 10^{-4}$
$CO_2$ viscosity (Pa · s)	$7.2 \times 10^{-5}$	$6.2  imes 10^{-5}$	$5.0  imes 10^{-5}$	$4.2 \times 10^{-5}$
Water density (kg/m <sup>3</sup> )	994	990	986	980
$CO_2$ density (kg/m <sup>3</sup> )	815	735	645	535
Interfacial tension (mN/m)	36.0	34.5	33.4	32.7
log(Ca)	-3.40	-3.53	-3.73	-3.87
log(M)	-1.01	-0.99	-1.01	-1.02

LBM lattice, probability function and directions,

(Gooya et al., 2019)

<sup>2</sup>D case



#### Porous medium models, viscosity ratio of 8.427



0 ts





7100 ts

Water in blue,  $CO_2$  in red



Water in blue,  $CO_2$  in red

#### Porous medium models, comparison at same timestep



Viscosity ratio of 1



Viscosity ratio of 8.427



## Conclusion

- Pseudopotential LBM was applied to the problem of modeling CO<sub>2</sub> sequestration, achieving stable models and giving useful insight into parameters. Domain verification was applied and confirmed grid independence of the model.
  - Validation test using channel model
  - Porous medium model at 1:1 viscosity and 8.427:1 viscosity done
  - Grid verification performed



#### Future work

- Capture more details of CO<sub>2</sub> and H<sub>2</sub>O interaction featuring both density and viscosity ratios
- Adaption of Peng-Robinson and crossover EoS models, which capture more physics of fluids