Lattice Boltzmann Modeling of Gaseous Diffusion in Unsaturated Porous Media Under Variable Gravity Conditions

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Introduction

- NASA is considering growing plants as part of a bioregenerative life support system to supply food and recycle cabin gases and water for long duration space missions.
- Reduced gravity (µg) conditions aboard orbiting space craft (i.e., International Space Station) present a challenge for management of porous media water and oxygen supply to plant roots.
- Differences in fluid distribution under µg affect gas diffusion and may affect plant growth.
- Prohibitive costs of experiments and the need for detailed models linking liquid distribution to diffusion with and without gravity make the Lattice Boltzmann method (LBM) an ideal modeling tool.

Objectives

1. To characterize liquid distribution in porous media under zero gravity (0g) & earth's gravity (1g).
2. To quantify gaseous diffusion coefficient as a function of water content for 0g and 1g.
3. To identify the effect of microgravity on gaseous diffusion.

Lattice Boltzmann Method

- A descendant of cellular automata; reproduces macroscopic fluid dynamics without resolving the forces applied to each particle.
- Particle distributions at each node **x** relax according to

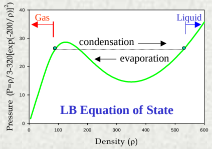
$$f_a(\vec{x}+\vec{e}_a, t+1) = f_a(\vec{x},t) - \frac{1}{\tau}[f_a(\vec{x},t) - f_a^{eq}(\vec{x},t)], \quad a = 0,\ldots,8$$

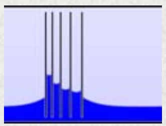
- Two different modeling approaches (and distinct codes) were used for each simulation.

Single-component, multi-phase code – Liquid modeling

(One fluid with non-ideal equation of state.)

- Used to find equilibrium position of liquid in idealized porous medium.
- Gravity parameter was calibrated by simulation of capillary rise.





Multi-component, single-phase code – Gaseous diffusion modeling

(Two fluids, both with ideal equations of state.)

- Used to simulate gas diffusion through porous medium.
- Ability of code to simulate diffusion was testing by comparison with analytical solutions.

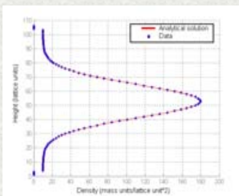
Initial condition | 200 timesteps | 1000 timesteps | 20,000 timesteps

corresponds to

$$C = \frac{C_0}{\sqrt{4\pi D_0 t}} \exp\left[-\frac{(x-2na)^2}{4D_0 t}\right],$$

$$for \quad n = 0, \pm1, \pm2, \ldots$$

- Intrinsic diffusion coefficient D_0 was calculated by fitting analytical solutions; the resulting value of D_0=0.175 was consistent over several different diffusion geometries.



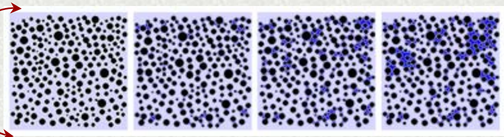
Numerical Experiments (LBM)

Using two lattice Boltzmann codes, we simulated gas diffusion under 1g and 0g at varying water contents. Each simulation was performed in two steps.

Single-component, multi-phase LB – Equilibrium Liquid Distribution

Apply density boundary conditions to gas-filled porous medium and allow liquid to condense in pore spaces.

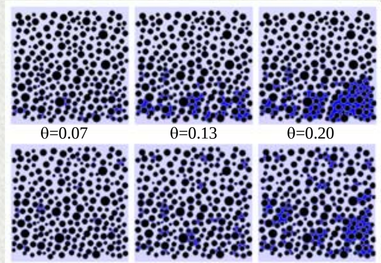
Density boundaries



Periodic boundaries

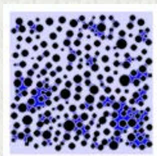
Initial Condition | 20,000 timesteps | 100,000 timesteps | 1,000,000 timesteps (equilibrium)

Vary density boundary conditions to attain different values of equilibrium water contents.

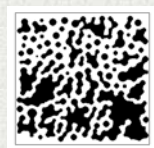


Multi-component, single-phase LB – Gaseous Diffusion with fixed Liquid Distribution

Assume diffusivity of gas in liquid and diffusivity of gas in solid are negligible; i.e., $D_{g\text{-}l} = D_{g\text{-}s} = 0$.



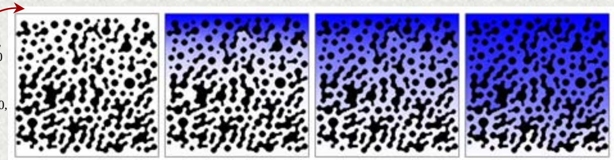
Convert liquid nodes to solid defining effective diffusion pathways for a particular liquid content



Use converted image as initial condition for diffusion simulations.

C_{white} =10, C_{blue}=1000

C_{white} =1000, C_{blue}=10



Periodic boundaries.

Initial condition | 20,000 timesteps | 70,000 timesteps | 850,000 timesteps (equilibrium)

Measure steady-state flux *q* through domain & calculate effective diffusion coefficient as: $D_{eff} = -\frac{q}{dC/dz}$

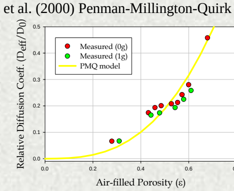
Results

- Results show good agreement with the Moldrup et al. (2000) Penman-Millington-Quirk model.

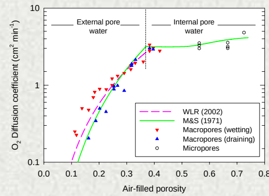
$$D_{rel} = 0.66\Phi\left(\frac{\varepsilon}{\Phi}\right)^{(12-m)/3}$$

where ε is air-filled porosity, Φ is porosity, and m is a fitting parameter.

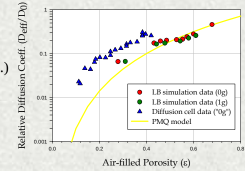
We found m=3.5 to give the best fit.



- Lower diffusivities in 1g due to blockage of diffusion pathways by saturated bottom layer.



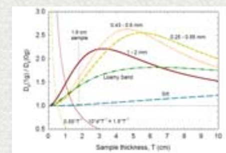
- Jones et al. (2003) used a flat horizontal diffusion cell filled with a coarse-textured plant growth medium to measure gas diffusion with minimal gravitational effects.
- Millington and Shearer's (1971) dual-porosity diffusion model was used to fit both micropore and macropore data.



- Comparison with experimental data shows our simulation results to be qualitatively correct and reasonable. (Only the macropore region is considered.)
- Differences are attributable to:
  - ➢horizontal vs. vertical diffusion orientation
  - ➢effects of domain thickness
  - ➢different pore size distributions

Conclusions

- LBM simulation results are in good agreement with established models and experimental data; hence they offer a means for studying fluid behavior under variable gravity to assist with root module design and porous media selection as a first step before engaging in expensive and time-consuming experiments in space.
- LBM results confirm the dominance of capillary forces under microgravity, resulting in a more uniform water content distribution than in 1g.
- In earth's gravity we observe higher water contents at the bottom of the sample due to interplay of gravitational and capillary forces, resulting in lower vertical gas diffusion in 1g relative to 0g simulations.
- Excluding the bottom water-saturated layer for vertical diffusion or for horizontal diffusion we expect higher diffusion coefficients for 1g than for 0g (Jones et al., 2003)



Future Work

Effect of gravity on gaseous diffusion in unsaturated porous media remains inconclusive due to limited domain size (finite number of diffusion pathways) and lack of experimental data. We are currently running simulations in larger domains to reduce domain size bias. An experimental system is scheduled to be launched to the ISS in Fall 2005 to obtain definitive measurements in a range of unsaturated porous media (NASA-ORZS project).

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Acknowledgments

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