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Density Profile and Flow of Miscible Fluid with Dissimilar Constituent Masses

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Abstract

A computer simulation model is used to study the density profile and flow of a miscible gaseous fluid mixture consisting of differing constituent masses ($m_A = m_B/3$) through an open matrix. The density profile is found to decay with the height $\propto \exp(-m_{A(B)}h)$, consistent with the barometric height law. The flux density shows a power-law increase $\propto (p_c - p)^\mu$ with $\mu \simeq 2.3$ at the porosity $1 - p$ above the pore percolation threshold $1 - p_c$.

1 Introduction

Understanding the flow of a complex gaseous mixtures, sedimentation, and evolution of density profiles of its constituents in geo-marine systems and near-surface ecological environments is becoming increasingly important [1, 2]. There are a number of examples: (i) High density brines associated with salt tectonics in large salt provinces (e.g. the Gulf of Mexico) have been breaching the seafloor and forming pools toxic to native flora and fauna [3]. This involves flow of a mixture of fluids with different densities due to different salt content and temperature. (ii) A mixture of air and radon flux through unsaturated soils within the upper few meters of the land surface. Radon 222, one of the intermediate products of the decay of uranium 238 to lead 206, is an odorless, radioactive gas (with half life 3.8 days), and is common in many soils and rocks. Because radon is about 8 times more dense than air, and is relatively inert [4], it easily penetrates porous building materials in ground floors and basements, especially when pressure gradients are created by central heating systems [5]. The U.S. Environmental Protection Agency (EPA) estimated in 1986 that 5,000 to 20,000 persons in the United States die of lung cancer each year from inhaling radioactive radon decay products in homes and buildings [5]. (iii) Evidence of methane hydrate formation below the ocean floor and in sub-ocean bottom in mud-volcano involves the flow and sedimentation of complex gas and fluid mixtures with dissimilar masses [6, 7, 8]. Studies of flow and density distribution of a mixture of miscible gas and fluids through porous media are therefore highly desirable.

Systematic studies based on the field measurements of flow and density profile of gas and fluid constituents in geomarine environment are severely limited [6] due to uncontrollable changes in geothermal parameters and morphological variations. Thus, computer simulation studies remain one of the most viable tools to probe such difficult issues as flow [9, 10, 11] and density profile [12]. Incorporating all details (multiple constituents and their characteristics) even with a coarse grained host matrix i.e. open porous media with appropriate concentration gradient and pore distributions [6] is a challenging issue. Lattice gas and particulate methods in general (Boltzmann, Cellular Automata, Ising (interacting), etc.) [13, 14] have been used in diverse applications of fluid flow. In study of the density profile and fluid flow of an interacting fluid mixture through porous media, a direct application of traditional hydrodynamics approaches [15, 16] becomes intractable; apart from a major problem of enormous boundary conditions in such a porous medium

(percolating system), it is not clear how to include interaction or reaction between the fluid components in hydrodynamic equations. Interacting lattice gas [12] may be a simple approach to initiate probing such difficult issues.

Very recently we studied the flow of a fluid described by particles, say of type "A" through an open porous medium using a computer simulation model [17]. The porous medium is generated by a random distribution of sediment particles of concentration p on a simple cubic lattice. The bottom layer of the matrix is connected to a source of mobile fluid particles ("A"). As soon as a bottom site becomes empty, it is immediately filled by a particle "A" from the source. Particles in the bottom layer are not allowed to move below this plane due to presence of abundant source particles. On the other hand, the particles can escape the system from the top if they attempt to move to the higher layer. In this concentration driven system, the flux density shows a power-law decay with the porosity near percolation threshold. The steady-state density profile of fluid particles depends systematically on the barrier concentration p .

In this article, we extend our previous studies [17] to a miscible two-component system consisting of constituents, say "A" and "B" with dissimilar masses (m_a and m_b , $m_b = 3m_a$). The model is described in the following section 2. We incorporate the effect of gravitational potential energy in moving the particles and allowing them to escape the system from the bottom layer as well. The injection probability of particles A and B at the bottom remains equal. The results are presented in section 3 with a conclusion in section 4.

2 Model

Each site on a simple-cubic $L \times L \times L$ lattice, with L up to 250, can be in one of four states: occupied by an A particle, occupied by a B particle, empty (0), or a barrier site. Nearest-neighbor particles interact with energy J such that A and B mix well: $J(A, A) = J(B, B) = -J(A, B) = -J(B, A) = -J(A, 0) = -J(B, 0) = 1$ where negative J means attraction and positive J means repulsion. The immobile barriers exert no force on the particles except to prevent them from occupying the barrier site. The energy thus is

$$E = \sum_i \sum_k J(I, K)$$

where i runs over all particles, k over all neighbor sites of i , and I and K are the corresponding site variables (A, B, barrier, or 0).

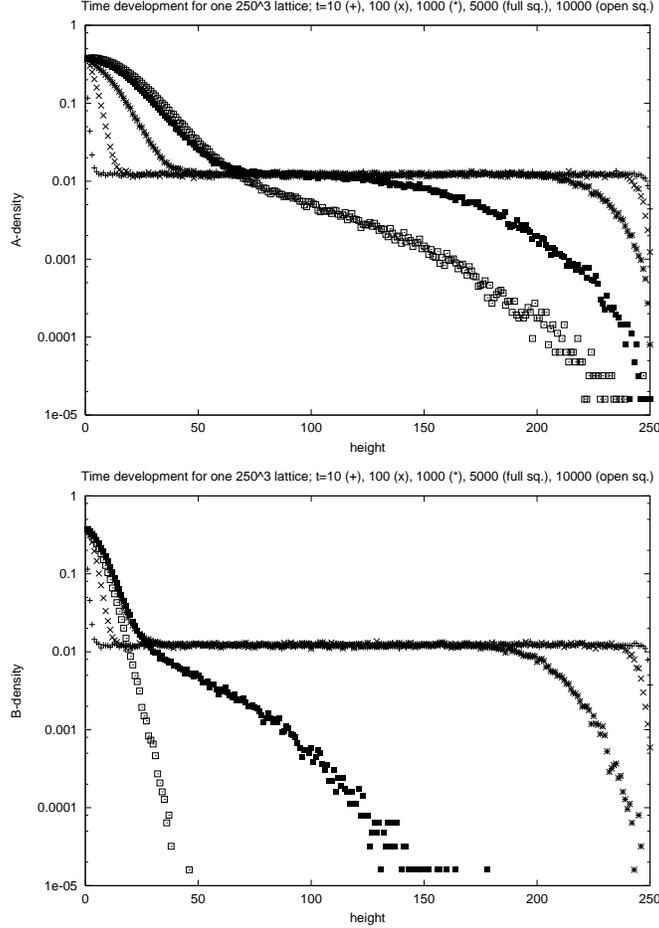


Figure 1: Crossover from constant to exponential density profiles, with increasing times t as given in headline, for A-particles (part a) and B-particles (part b). No sites are barriers in this simulation.

A and B particles can move with a Metropolis probability $\exp(-\Delta E/k_B T)$ to neighboring sites; here ΔE is the energy change associated with this move and $k_B T = 5$ is the thermal energy. If a particle on the lowest plane moves upwards or horizontally, we inject a new particle A or B (with equal probability) onto the vacated site. If a particle on the lowest plane wants to move

downward, it drops out. A particle moving upward from the highest plane (relatively a rare event) is lost, without any injection from the top. Periodic boundary conditions are applied in the horizontal directions. In this way, an $\infty \times \infty \times L$ plate is approximated, with new material injected from the bottom at a nearly constant rate.

Gravity pulls down the particles through an energy $mk_B T$ where the lattice constant and the gravitational constant are incorporated into the dimensionless mass $m = 0.1$ for A and $m = 0.3$ for B particles. Thus the barometric height law gives an equilibrium density $\propto \exp(-mh)$ as a function of height h , $1 < h < L$.

One time step is an attempt to move each particle once (on average) through random sequential updating; it does not matter much if instead we enforce exactly one attempt per particle for each time step. For $L = 30$ we used up to $t = 10^6$ time steps, without seeing any long-time effects; for larger L (50 to 250) typically $t = 10^4$ to 10^5 gave equilibrium. Initially, the lattice is occupied homogeneously with a low concentration of particles, half A and half B. Our computer program allows many more choices for interactions and boundary effects and is developed to investigate many different systems (details are available from ras.pandey@usm.edu). One diffusion attempt, without barrier sites, took about 0.5 microseconds on one Cray-T3E processor.

3 Results

Fig.1 shows for our largest lattices how the initial constant density profiles change with time, starting from the two boundaries, into a roughly exponential decay for intermediate heights. The equilibrium density profiles, Fig.2, at intermediate densities are consistent with the barometric height law shown as straight lines in these semilogarithmic plots, both with and without barrier sites. The nearest-neighbor correlation functions (not shown), i.e. the number of A or B particles surrounding a particle at height h , decay qualitatively similar to the density profiles.

Fig.3 shows as a function of the barrier concentration p the system's permeability, defined as the net flow (per unit time and unit cross-sectional area) at the top or bottom surfaces divided by the injection rate at the lowest plane. The straight line in this log-log plot suggests a power law similar to that of the electrical conductivity in random resistor networks. Fig.4 shows

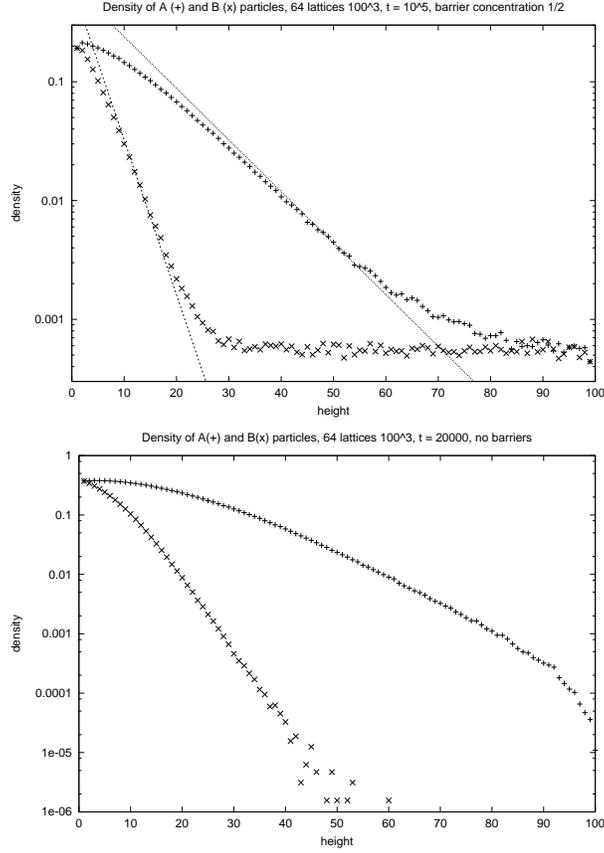


Figure 2: Equilibrium density profiles with (part a) and without (part b) half the sites occupied by barriers. The straight lines are $\propto \exp(-mh)$.

the density profiles of the B particles for the same simulations. We see there an exponential decay, followed by a plateau whose value strongly increases with increasing p , suggesting a trapping of particles by the barrier sites. We have also looked at the velocity and instantaneous velocity profiles of the two constituents which are consistent with our expectations, i.e., more mobility toward the top.

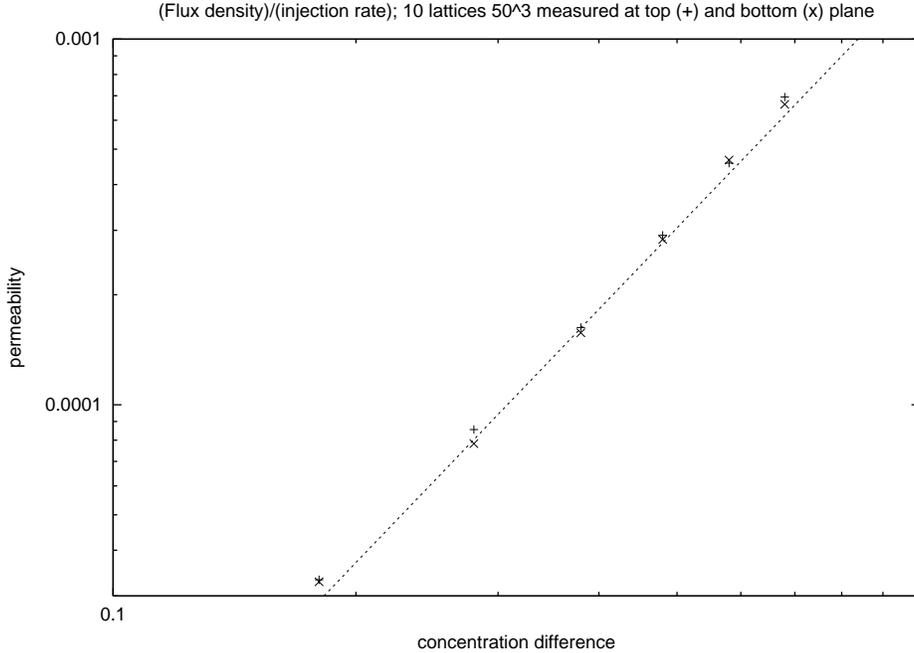


Figure 3: Double-logarithmic plot of permeability versus $p_c - p$ where $p_c = 0.6884$ is the percolation threshold and p the barrier concentration. For $p > p_c$ there is no infinite connected set of fluid sites between the barriers and thus the permeability vanishes. The straight line has a slope 2.3.

4 Conclusion

A computer simulation model is used to study the flow rate, sedimentation, and density profile of a mixture of miscible particle systems for a range of porosities above the pore percolation threshold in an open porous medium. In our concentration driven system, the steady-state density profiles for both A and B fluid are reached. Both density profiles show the well-known exponential decay $\propto \exp(-m_{A(B)}h)$ with height h . The effect of mass difference is vividly illustrated in the density profiles: while for our lattice sizes the density of A particles continues to decay up to the top plane the density of B particles already saturates at some low value. The saturated density of B particles increases on decreasing the porosity $1 - p$ - we speculate this saturation is due to trapping of particles in the pores.

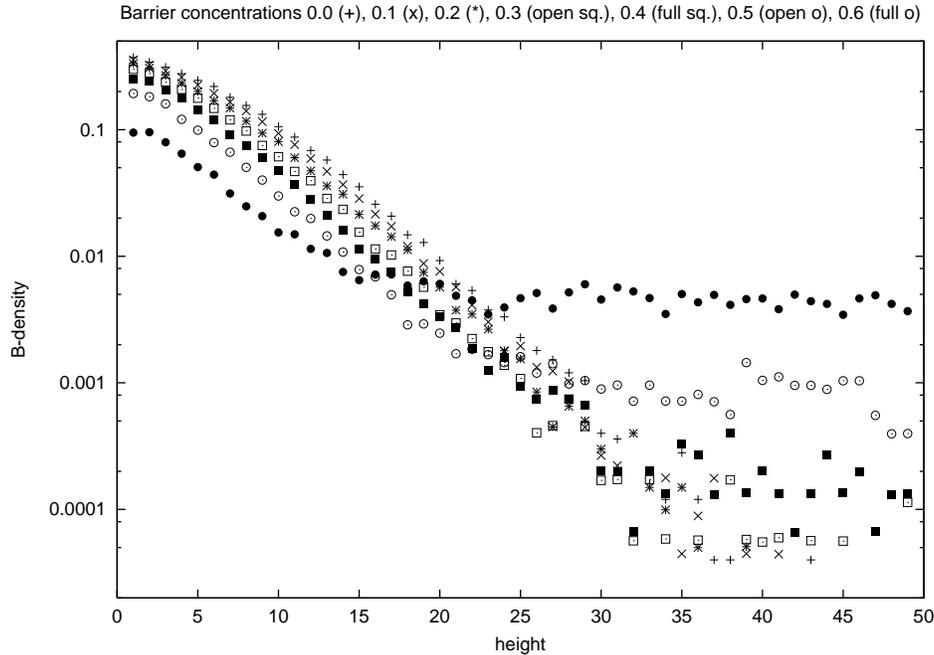


Figure 4: Equilibrium density profiles of B-particles for various barrier concentrations (same simulations as for Fig.3).

The flux of particles A at the bottom becomes equal to the outward flux from the top in steady state. The flux density of particles A decays with porosity with a power-law $\propto (p_c - p)^\mu$ with $\mu \simeq 2$.

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