

# Molecular Dynamic Study of Fluid Flow Through a Porous Medium

B. V. Costa: P. 2. Courat

*Departamento de Física, Universidade Federal de Minas Gerais*

*Caixa Postal 702, 30161-970 Belo Horizonte, MG Brazil*

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Molecular Dynamics of a two dimensional fluid flow through a porous medium is presented. Although the simulation is a crude representation of the experimental process we observe some qualitative agreement with the phenomena that occur in experiments.

## I. Introduction

The fluid diffusion through a porous medium under the action of an external field is of great applied importance from petroleum and chemical engineering to hydrology and chemical or nuclear waste storage. Recent catastrophes involving poisoned materials accidentally spread out on the Earth surface generated a great effort to understand the mechanism of how such a fluid penetrate the ground poisoning the underground water or a river in the neighborhood<sup>[1-7]</sup>. At the mesoscopic level the fluid flow through a porous medium depends on the detailed structure and geometry of the pore space. The presence of the solid part of the medium forces the streamlines to meander through the pore volume giving rise to a distribution of path lengths. The streamlines through one pore may separate into different pores and also meet again in a later pore. The velocity along a single streamline also fluctuates being slow through narrow pores and in stagnant regions, and faster than the average flow in wide pores oriented parallel to the average flow. The particles in the fluid which are carried by the streamlines from one pore to another appear to be effectively performing random walks through the medium<sup>[8,9]</sup>. The conventional classical mesoscopic description of such a phenomenon is provided by the convection-diffusion equation<sup>[1-4]</sup>

$$\frac{\partial C}{\partial t} = \vec{\nabla} \cdot (\mathbf{D} \cdot \vec{\nabla} C - \vec{U} C), \quad (1)$$

where  $C(\vec{r}, t)$  is the fluid concentration and the dispersion tensor  $\mathbf{D}$  depends in general on the flow velocity  $\vec{U}$ . Numerical solutions of eq. (1) can provide some insight into this problem since a suitable calculation gives a detailed description at the mesoscopic level through which the process evolves. However, the amount of required computer time easily becomes prohibitively long if the sizes of the simulated systems become large. Therefore, computer calculation of flow through a porous medium have so far taken a simplified approach, describing the fluid as a continuous. The flow is governed by eq.(1) which supplemented by a number of boundary conditions, are solved by finite-element methods<sup>[10]</sup>. In this paper we present a molecular dynamics (MD) simulation of the fluid flow through a porous rigid medium. Our simulation allow us to study the system at a molecular level. The system we study is chosen to be reasonably simplified in order to limit the intrinsic complexities of the process and to keep the required amount of computer time within reasonable limits. For example, our simulations are carried out in two dimensions and contain two types of particles which interact via a Lennard-Jones potential. Although such limitations prevent a quantitative comparison between simulational and experimental data, it is expected that many qualitative features observed in our simulations occur in the actual experiments as well.

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\*bvc@fisica.ufmg.br

†pablo@fisica.ufmg.br

## II. The computer experiment

The system we want to simulate consists of a rigid substrate -the porous medium- and a fluid initially just over it, which is allowed to penetrate in the substrate under the action of a field  $\vec{g}$  in the  $-y$  direction (See Fig. 1). The substrate was created by distributing at random particles on a triangular lattice in such a concentration that the fluid may percolate. For the initial fluid configuration we distributed randomly the particles just above the substrate as shown in Fig. 1. Periodic boundary condition were assumed in the  $x$ -direction throughout the simulations. All particles in the system interact with each other through a Lennard-Jones (LJ) potential

$$U(r) = \epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right] \quad (2)$$

The potential  $U$  is spherical so that it depends only on the interparticle distance  $r$ . A repulsive part prevents particle-particle imploding while the attractive part binds one to the other. Roughly  $a$  is the particle hard core diameter. The potential has a minimum at  $r = 1.15\sigma$ . We use different values for  $a$  and  $\epsilon$ , depending if the interaction is between fluid-fluid (f-f) or fluid-substrate (f-s) particles. Their values were arbitrarily chosen as  $\epsilon = 1.0(1.5)$  for f-f(f-s) interactions and  $a = 1.0(3.0)$  for the fluid (medium) hard core. There is no real loss of generality in such a choice since all quan-

tities are rescaled by  $\epsilon_{f-f}$  and  $\sigma_{f-f}$ . In our simulation particles do not interact if their distance is larger than  $3\sigma$ . Without such a cut-off, the simulation would be prohibitively slow. All the simulations are of molecular dynamics type which means that the particles move according Newton's equations of motion which can be easily derived from the Hamiltonian

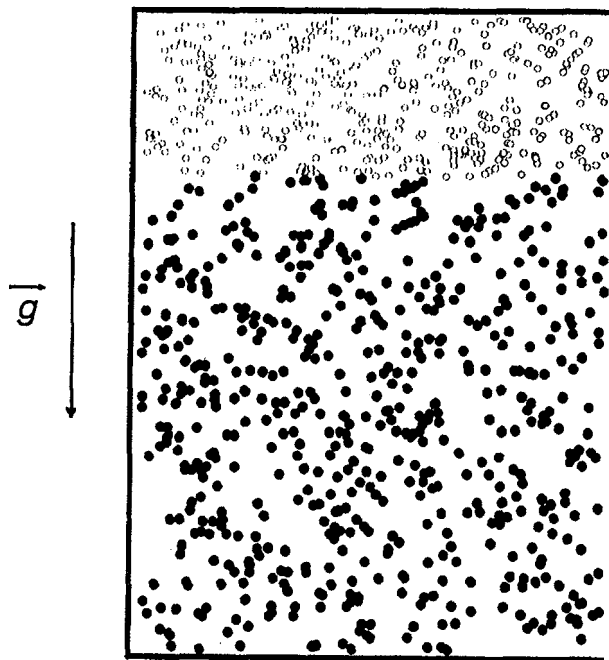


Figure 1. Initial condition used in our experiment. Open circles are fluid particles and full circles are particles in the solid porous medium.

$$H = \sum_{i=1}^{N_f} \frac{p_{fi}^2}{2m_{fi}} + \sum_{i<j}^{N_f} U_{f-f}(r_{ij}) + \sum_i^{N_f} \sum_i^{N_s} U_{f-s}(r_{ij}) + g \sum_{i=1}^{N_f} m_{fi} y_{fi} \quad (3)$$

and the Hamilton's equations

$$\frac{\partial H}{\partial r_{\alpha i}} = - \cdot p_{\alpha i} \quad \text{and} \quad \frac{\partial H}{\partial r_{\alpha i}} = - \cdot r_{\alpha i}, \quad (4)$$

where  $N_f$  and  $N_s$  are respectively the number of particles in the fluid and in the porous medium.  $r_{ij}$  is the distance between particles  $i$  and  $j$  and  $r_{\alpha i}$  ( $\alpha = 1, 2$ ) represents the coordinates  $x_i$  and  $y_i$ . Observe that there is no a kinetic energy term associated with the parti-

cles in the porous medium, as mentioned before they are considered as static. The equations of motion were solved by using a fourth order leap-frog scheme with small time steps  $\Delta t = 0.004\sigma \sqrt{m_f/\epsilon_{f-f}}$  ( $m_f$  is the mass of a particle in the fluid.). Before we go on with the simulation we need an estimate of the solid-fluid phase transition temperature ( $T_{s-l}$ ) for the system we use. Therefore, we carried out an independent simulation of a liquid strip with periodic boundary condition

in one direction and open in the other. In order to determine  $T_{s-l}$  we started with a solid with 1200 particles at very low temperature. By solving the equations of motion we evolved the system measuring the velocities of the particles ( $v_i$ ) from time to time. Of course the mean velocity  $\langle v^2 \rangle$  is related to the temperature of the system by the equipartition theorem<sup>[11]</sup>

$$k_B T = \frac{1}{2} m_f \langle v^2 \rangle = \frac{1}{N_f} \sum_{i=1}^{N_f} \frac{1}{2} m_f v_{fi}^2 . \quad (5)$$

By renormalizing velocities we may control the system's temperature. At  $T_{s-l}$  the internal energy should show a jump which is just the latent heat associated with the solid-liquid transition. In Fig. 2 we show a plot of our results for three different initial conditions of energy versus temperature. We observe the strip to freeze at  $T = 0.40$ , fragment and starts to evaporate around  $T = 0.45$ . The arrow in Fig. 2 shows our estimate for  $T_{s-l}$  ( $\sim 0.43$ ). Here, temperature is measured in units of  $k_B/\epsilon$  where  $k_B$  is the Boltzmann's constant. Of course, this is not an accurate estimate of the critical temperature but was good enough for our purpose, since we worked above  $T = 0.45$ . The number of particles we have used in our simulations was 1500 in the solid distributed over an rectangle with sides  $L_x = 20$  and  $L_y = 30$ . For the fluid we have used 800 particles initially distributed in a region of sides  $L_x = 20$  and  $L_y = 5$ .

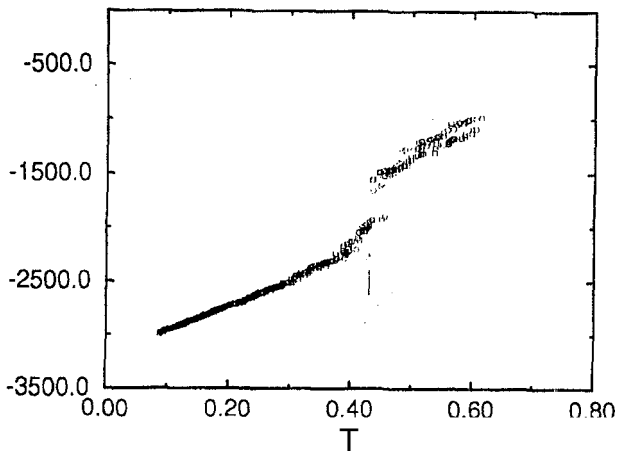


Figure 2. A plot of the internal energy versus temperature for a Lennard-Jones system with periodic boundary condition in one direction and open in the other. The arrow shows the solid-liquid transition temperature. Units are defined in the text.

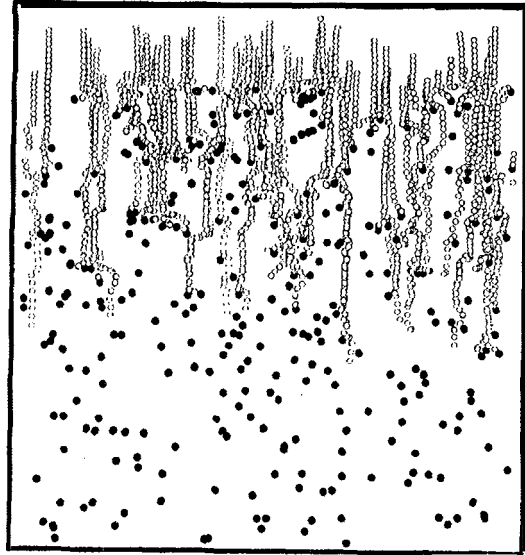


Figure-3a. A cumulative picture. We have used 104 time steps. 200 solid particles and 50 fluid particles to compose this picture. It shows the streamlines through the pore volume.

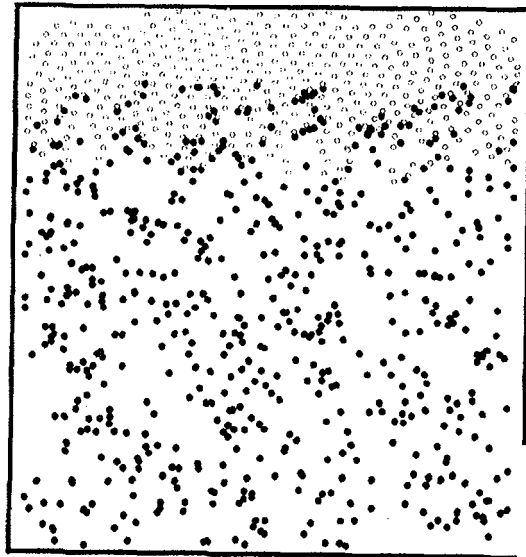


Figure-3b. Final configuration of a simulation where we have used 103 time steps. 800 solid particles and 200 fluid particles.

### III. Results of the simulation

We measured two aspects of the fluid flow: the front flow pattern velocity and the pattern rugosity. Typical flow patterns are shown in Figures 3a-b and 4a-b. Figure 3a and 4a are cumulative pictures and they show the channels from which fluid particles go along. Figures 4a-b show configurations after  $10^3$  and  $10^4$  time

steps respectively. The full circles are particles of the solid porous medium while open circles are fluid particles. In Fig. 4a at the central region where the substrate presents a higher density we can see that the fluid particles cannot penetrate so easily as in the border where the density is lower. In fact even for longer times we did not observe fluid penetration since it wets the substrate which becomes impenetrable for the fluid. Figure 5 shows the profile rugosity as a function of time. It is calculated as the fluctuation  $\rho = \langle (\langle y \rangle - y)^2 \rangle$ , where  $\langle y \rangle$  is the averaged distance of fluid particles to the inferior face of the solid at  $y = 0$ . It starts from  $\rho(t = 0) = 0$  reaching some constant value after a long enough time. Figure 6 shows the profile velocity. It is calculated as the velocity of the center of mass of the fluid inside the porous medium. The initial velocity of the particles are chosen at random directions but in such a way that the fluid temperature is about 0.50. After each 50 time steps we renormalize velocities to maintain the temperature as 0.50 it means that the substrate works as a heat reservoir.

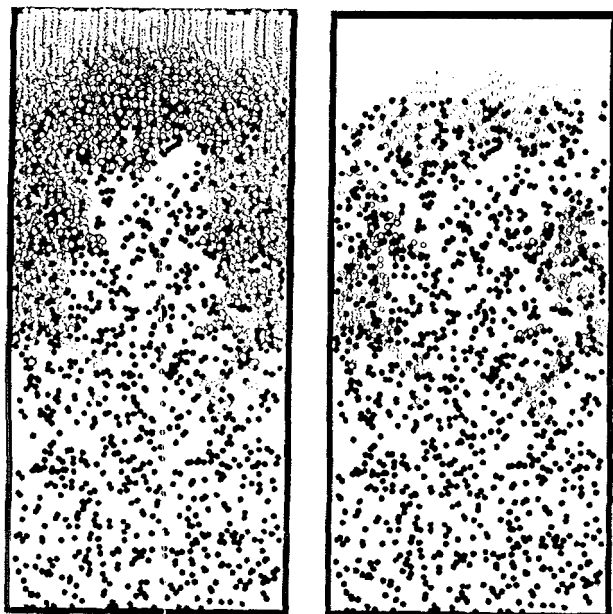


Figure-4a. A cumulative picture after 104 time steps. We have used 1500 solid particles and 100 fluid particles. Figure-4b. Final configuration corresponding to the simulation in figure 4a.

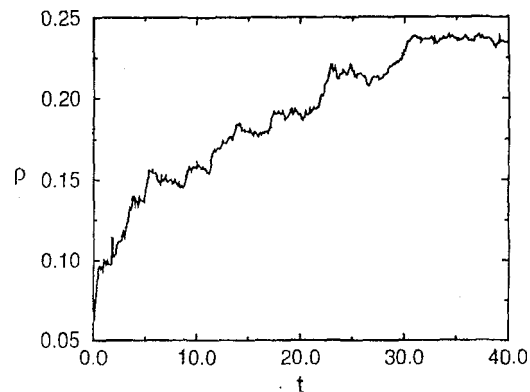


Figure 5. The rugosity as a function of time. We have used configurations of 1500 solid particles and 200 fluid particles.

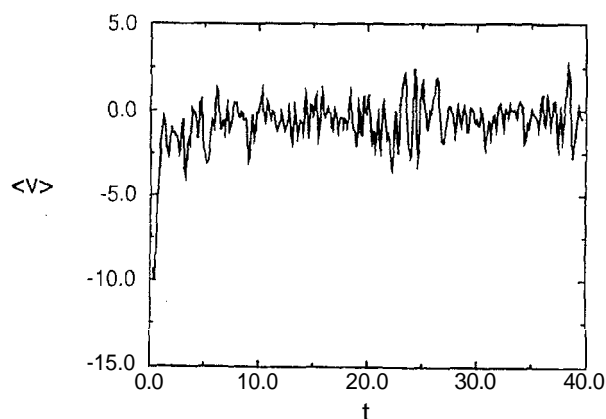


Figure 6. The averaged velocity as a function of time. The number of particles is the same as in the figure 3.

#### IV. Conclusion

Our simulations show the possibility of performing molecular dynamics simulation of fluid flow through a porous medium. Although the simulations are not able to closely model the experiments and hard to compare quantitatively we observe some qualitative agreement with the phenomena that occur in experiments. The streamlines may separate into different pores and also meet again at a later pore. Fluid particles are slow, or even may bind in regions where the solid medium is more dense. The velocity and rugosity distribution as a function of time relax to their equilibrium values for long times. Such qualitative results show that molecular dynamics simulations may be a very useful tool to understand the fluid flow through porous medium. It would be interesting to test the results of the simulation against mesoscopic finite elements calculations. We are now extending our simulations to three dimensional systems and boundary conditions where the fluid is forced against the surface of the porous medium by

a pressure field as in the process of water injection in oil wells.

### Aknowledgments

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