MOLECULAR DYNAMIC SIMULATION OF THE FLUID
CONCENTRATION FLUCTUATIONS IN TWO DIMENSIONAL
POROUS MEDIUM

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Abstract. The filtration of fluid in 2D porous medium is simulated by the
molecular dynamics technique. The high concentration of fluid is created at
the initial point in time and the number of fluid particles is investigated in
all porous. The concentration of particles pores and parameters of interac-
tion potentials is varied. In all cases the particles concentration decay is well
described by exponential functions. The decreasing of the interpore channels
leads to the increasing of the relaxation time and does not depend on the
system size. This phenomenon is observed in real filtration processes.

In recent years, much attention has been devoted to the problem of description
the non-stationary filtration in porous mezo and macro structures [1, 2]. In this
paper the evolution of density fluctuations is considered by the molecular dynamics
simulation [3, 4]. The density of particles is related by fluid or gas pressure in
modeling 2D porous media.

The particles of solid state porous matrix interacting each other by means of
Lennard and Jones potential

\[ U(r) = 4\varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right] \]

and particles of fluid interacting each other and with particles of porous matrix
via potential

\[ U = \alpha (r - \rho)^2 \]

where \( r \) – the distances between particles, \( \varepsilon = 1, \sigma = 2^{-1/6} \), parameter \( \alpha \) varies
from 0 to 100, \( \rho \) varies from 0 to 1. The mass of all particles was equal to unity
\( m=1 \).

2D porous system is constituted of the square lattice with porous cells. The
particles of solid state matrix embedded at sites in the lattice. In the borders of
the system under considerate are positioned the fixed particles. The parameters \( \alpha \)
and \( \rho \) are adopted so that matrix particles hesitate near the equilibrium position.
The matrix particles simulate the compressibility and elastic waves propagation in
porous medium. The average distance between them was equal to unity. Into a
pores was and transferred a fluid particles. The potentials [1] and [2] imitated the
situation when the fluid particles move in pores and inter pores channels and have
a translation agility.

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In our computer simulation the considerable fluctuation of the particles number produced in pore with index (1,1). Other pores have more less number of particles in this time moment. Then the processes of redistribution of fluid particles between pores begin.

First the number of particles increase in pores (1,2), (2,1) and (2,2) then in (1,3), (3,1), (3,2) and etc. At last the quasi equilibrium state is established in all pores. Then we vary the size of systems and the concentration of particles in pore (1,1).

In Fig.1 is shown the time dependence of particles number in pore (1,1). The first curve is associated the condition when the concentration in pore (1,1) was more than in others 3 times, the second curve 15 times and the third curve 81 times ones. It is easily to seen that in all cases the kind of decay of the number of particles in pore (1,1) is similar and may be described by exponential type function

\[ N(t) = N_0 \exp \left( -\frac{t}{\tau_{\text{char}}} \right) \]

where \( N(t) \) – the number of particles in current time moment, \( N_0 \) – in initial time moment ones, \( \tau_{\text{char}} \) - characteristic time of decay the elevated density of the particles number in pore. The number of particles is normalized to the maximal number. In Fig.1 are shown the exponential approximations by solid lines also. \( \tau_{\text{char}} \) in our experiments varies from 1 to 100.

In other pores are observed the increasing of particles density. Next the density is reduced as the initial indignation penetrates deep into system. This process is shown in Fig.2 for the pores (1,2), (2,2) and is compared with pore (1,1). We see that the maximum of particles is observed in pore (1,2) at \( t=2.5 \) and in pore (2,2) at \( t=5 \). Then the perturbations transfer into pores (1,3), (2,3), (3,3) etc.

It is an interesting to know what will be happen if we have narrowed the inter-pore channels. We may do it varying the potential parameters and increasing the repelling forces between matrix particles and fluid particles ones. This procedure will be imitate the narrowing of the inter channels distances. Then the permeability of porous medium will reduce. Let us denote as \( \rho \) the characteristic radius of the repelling force in potential \( \Phi \). This quantity may be named as effective width of the interpore leaking field. We expect that characteristic time \( \tau_{\text{char}} \) will be increasing when the \( \rho \) rise. Such is indeed the case in our experiments. In Fig.3 is demonstrated the dependence of \( \tau_{\text{char}} \) from \( \rho/r_{\text{max}} \) for the pore (1,1). Here \( r_{\text{max}} \) is the one half of the distances between the nearest neighbor matrix particles and \( \rho/r_{\text{max}} \) may be named as relatively width of the field interpore leaking. All the other parameters in this kind of computer simulation are fixed. We see with growing of the \( \rho/r_{\text{max}} \) the filtration resistance becomes essential and the \( \tau_{\text{char}} \) considerably increase. This fact we may interpret as the decreasing the piezoconductivity when the permeability decreases also. Experiments shown that the size of system does not influence essentially on the value of \( \tau_{\text{char}} \).

### Conclusion

In our computer experiments the decay of the concentration of the particles in separate pore is well described by exponents. This leads to the validity of relaxation theories \[ [1] \]. The time of relaxation does not depend on the size of the system. The increasing of the repelling forces between the fluid and matrix particles tends to
MOLECULAR DYNAMIC SIMULATION

increase the time of relaxation of fluid particles in pores, what corresponds to the growing of filtration resistance.

References

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Figure captions

Fig.1. The time dependence of the particles number in pore (1,1). The density of the particles in pore (1,1) more than in others 3 times (curve 1), 15 times (curve 2), 81 times (curve 3).
Fig.2. The time dependence of the number of particles in pores (1,2), (2,2) and (1,1).
Fig.3. The dependence of the characteristic time of particles density decays in pore (1,1) from effective width of the leaking field.

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Fig. 1
Fig. 2
Fig. 3