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2D SIMULATIONS OF LIQUID PERCOLATION THROUGH MODEL POROUS MEDIA: PRELIMINARY MD AND DPD RESULTS

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Abstract: In the paper we make a short overview of computer models based on particle approach, which can be suitable for the simulation of fluid flow through porous media. We concentrate on Molecular Dynamics (MD) and Dissipative Particle Dynamics (DPD) methods. We describe main features of our simulation programs, and present and discuss preliminary results of MD and DPD simulations of 2D fluid flow through a simple model rigid porous media. The paper aims at the evaluation of the applicability of MD and DPD methods for simulations of liquid flows in media of complicated geometry.

Keywords: 2D flow simulations, particle methods, molecular dynamics, dissipative particle dynamics

1. Introduction

Numerical solution of fluid mechanics problems is a challenging task due to its wide theoretical and practical implications [1]. The classical approach is a continuum-based model described by the Navier-Stokes equations, which can be numerically solved using Finite Elements Method (FEM) or Finite Differences Method (FDM). This model is very powerful, but may be extremely difficult to use for complex systems, as those with time-dependent boundary conditions and/or with sediment granules added. Flow through porous media can be such a case, especially when granules forming the medium are of different shapes and sizes, can be deformed by the flow, can split or stick together. It may also be assumed that they act in a kind of chemical reactions with the fluid. With the above assumptions the continuous approach may face problems very difficult to solve.

An alternative approach, a particle representation of a fluid, can overcome many difficulties found in classical methods. The particle approach is a relatively recent development in the field of fluid flow modelling. Since it enables explicit continuous modelling of forces acting on molecules of fluid [2, 3], it seems to be a viable method to study flows under extreme conditions, to analyse the microscopic origin of flow instabilities, to find out what happens inside a boundary layer and to observe the flow of a molecular fluid in the micro-scale, where Navier-Stokes equations do not work any more.

First non-equilibrium molecular simulations applied to fluid flows appeared in the late 80'. They concerned the flow past an obstacle and eddy formation. The first simulations have been performed by Rapaport and Clementi [4], and continued by Cui and Evans [5]. A lot of work has been done to simulate formation of patterns of Rayleigh-Benard convection [6–11], flow of thin liquid films [12] and other. This new approach got a very strong impact in the last few years both in computational and theoretical aspects. Topics, such as convection, sedimentation, thermodynamic instabilities, developing of turbulence, flow in porous media, many-component flows, shock waves propagation and many others are of particular interest in particle models.

In this paper we give a short overview of particle methods suitable for simulations of fluid flows in porous media (Section 2), with particular attention paid to Molecular Dynamics (MD) and Dissipative Particle Dynamics (DPD) approaches. In Section 3 we describe the characteristic features of our programs. The simulation sample results are described and discussed in Section 4. Section 5 contains concluding remarks.

2. Particle methods for fluid flow through porous media – an overview

Let us describe in brief the general outlines of several particle methods that can be used for fluid flow simulation in a porous medium.

2.1. Molecular Dynamics (MD)

Molecular Dynamics has been first introduced for equilibrium systems [3, 13]. It is defined entirely by the properties of particles and their mutual conservative interactions. The particles are responsible for energy and momentum transport according to the rules of conservation. Each particle of an N-particle system interacts with all neighbours within a sphere with r_{cut} radius. Usually the interaction is defined as a two-body, distance dependent

potential function $U(r_{ij})$. An effective force $\boldsymbol{F}_i$ acting on particle i is defined as a sum of additive pair forces $\boldsymbol{f}_{ij}$:

$$\boldsymbol{F}_i = \sum_{j \in S(i, r_{cut})} \boldsymbol{f}_{ij}, \qquad \boldsymbol{f}_{ij} = -\nabla U(r_{ij}). \tag{1}$$

Particles motion is described by the Newtonian equations:

$$m_i \frac{d\boldsymbol{v}_i}{dt} = \boldsymbol{F}_i, \qquad \frac{d\boldsymbol{r}_i}{dt} = \boldsymbol{v}_i. \tag{2}$$

The MD simulations have been originally applied for computations of different parameters of gases, fluids and solids (such as diffusion coefficient, specific heat, electrical conductivity), and for investigation of material structure in micro-scale. For these applications, a great number of advanced MD algorithms have been developed [13]. The MD approach to a fluid flow modelling is, as mentioned in the introduction, a relatively recent development - the first non-equilibrium MD simulations of fluid flows started in late 80's.

Application of the "particle fluid" and description of the system dynamics directly by the Newton equations within the MD method enables:

- usage of the well known and numerically well defined simple, homogeneous mathematical model,
- taking into account the local density and anisotropy of the system,
- performing unconstrained simulations of shock phenomena,
- studying flows under extreme conditions,
- analysing the microscopic origin of hydrodynamic instabilities,
- getting insight into boundary layer phenomena,
- relating all the material properties to the particles and their interactions.

Relation of all physical properties to the particles solves a lot of numerical problems encountered in continuum models. MD approach allows:

- easy simulations of discontinuities of the system,
- self-adaptation of the system according to its physical nature (absence of grids),
- to avoid artificial loss of density on the boundaries,
- to eliminate many numerical difficulties concerning complicated boundary conditions.

By changing definitions of the particles and the potential, as well as by simple re-scaling of the equations of motion, the particle model may be applied for the description of flow and shock phenomena in dense liquids and solids in macro-scale. Assumptions concerning the change of interpretation are as follows:

- a macroscopic object is divided into N elements (quasi-particles),
- quasi-particles are large enough to interact only by a short range potential (described by quasi-potential) and small enough that local fluctuations do not change the object shape,
- system evolution is still described by the Newtonian equations.

Molecular Dynamics is a very straightforward and accurate, but also extremely time-consuming method. For classical MD simulations at least 10^5 particles in 2D are needed to observe hydrodynamic behaviours. One of the most promising approaches is DPD [13], which merges benefits of MD (in its re-scaled version) and Lattice Gas Automata [14] methods.

2.2. Dissipative Particle Dynamics (DPD)

Dissipative particle dynamics (DPD) is a relatively new particle approach introduced by Hoogerbrugge and Koelman [15], and developed significantly in the last few years [16–19]. The basic idea of the method is similar to that of MD. However, the particles here are not considered as atoms, but rather as mesoscopic clusters of physical particles. In this scale the total force acting on DPD particles consists of conservative (MD-type) interactions, a dissipative term responsible for viscosity, and a stochastic component which controls internal pressure and temperature. Similarly to the MD method, particles move in continuum space defined by positions $\boldsymbol{r}_i$ and momenta $\boldsymbol{p}_i$ for every particle ($i = 1, \lambda, N$). On the other hand, the system is updated in discrete timesteps δt in two phases: collision and propagation. This is similar to Lattice Gas Automata approach, as well as the event driven particle dynamics [7], where free time between collisions is greater than that in MD. In the collision phase the momenta change as:

$$\dot{\boldsymbol{p}}_i = \boldsymbol{p}_i + \sum_j \Omega_{ij} \boldsymbol{e}_{ij}, \tag{3}$$

where $\boldsymbol{e}_{ij} = (\boldsymbol{r}_i - \boldsymbol{r}_j)/\left|\boldsymbol{r}_i - \boldsymbol{r}_j\right|$ is the unit vector from particle j to i, while Ω_{ij} describes the momentum transferred from j to i. During the propagation phase, the particles move freely according to:

$$\dot{\boldsymbol{r}}_i = \boldsymbol{r}_i + \frac{\delta t}{m_i} \dot{\boldsymbol{p}}_i. \tag{4}$$

The interactions are limited to neighbours within a distance r_{cut} by assuming $\Omega_{ij} = 0$ for $\left|\boldsymbol{r}_i - \boldsymbol{r}_j\right| > r_{cut}$. Ω_{ij} depends not only on the distance between particles, but also on relative momenta expressed as $\left(\boldsymbol{r}_i - \boldsymbol{r}_j\right)\left(\boldsymbol{p}_i/m_i - \boldsymbol{p}_j/m_j\right)$. The expression for Ω_{ij} is usually applied in the form:

$$\Omega_{ij} = W\left(\left|\boldsymbol{r}_i - \boldsymbol{r}_j\right|\right) \cdot \left\{\Pi_{ij} - \omega_{ij}\left(\boldsymbol{p}_i - \boldsymbol{p}_j\right)\boldsymbol{e}_{ij}\right\}. \tag{5}$$

In (5) $\omega_{ij} = 1 - r_{ij}/r_{cut}$ is a positive coefficient responsible for dissipation of energy, dependent on relative momenta of neighbouring particles. $W(r)$ is a dimensionless, non-negative weight function. In the mesoscale it is sufficient to apply linear form of $W(r)$ decreasing and vanishing at r_{cut}: $W(r) = \left(3/(\pi r_{cut}^2 n)\right)(1 - r/r_{cut})$, where n is number density equal to N/V. $W(r)$ is a repulsive, MD-type component, while Π_{ij}, and $\omega_{ij}\left(\boldsymbol{p}_i - \boldsymbol{p}_j\right)\boldsymbol{e}_{ij}$ are stochastic, and dissipative terms, respectively.

2.3. Other particle methods

Although the results presented in Section 4 have been obtained within MD and DPD approaches, several other particle models suitable for simulation of complex fluid flows are briefly mentioned below.

The most important group of particle methods used for fluid flow is based on cellular automata approach, namely Lattice Gas Automata (LGA) and Lattice Boltzmann (LB) method. Actually LGA and LB models are much better established in the area of complex fluids than MD and DPD.

Lattice Gas Automata can be treated as a maximal simplification of molecular dynamics. The particles in LGA model can be placed only in the nodes of a mesh (usually hexagonal), and move from one node to another with unit velocity according to certain rules of interaction with the nearest neighbours, and conserving momentum and number of particles. The model has been first introduced in order to solve Navier-Stokes

equations by Frisch *et al.* [14, 20]. By introducing nodes, which cannot be occupied by particles, unmoveable obstacles forming porous medium are simulated. LGA method has been intensively used for simulation of particle fluid flow through porous material [21–24]. Due to its simplicity, the LGA model can have at least 10^2 times particles more than MD model, thus very large systems can be simulated.

Lattice Boltzmann method is an extension to LGA approach in the sense that it uses probabilistic particle distributions, rather than discrete particles [25]. The velocities are represented by floating-point values and the method is considerably less noisy than LGA. LB becomes now more popular in simulation of complex flows, in particular flows through porous media [26–28].

The **Hard Spheres model** was among the first computational methods that used particle approach for solving problems in hydrodynamics. It's not of much use now, at least in the original version. The method evolved into Granular Dynamics, which introduced particles that interact with each other only by direct contact with friction coefficients added.

Another method uses a **Particle in Cell** (PIC) [29] model with collisions. Because the particles in a typical fluid collide with neighbouring particles in a very short time ($\sim 10^{-14}$ s) from a macroscopic point of view, they do not conserve their energies and momenta during simulation, dissipating them among other particles in the proximity. Thermal quasi equilibrium is achieved in the same short time scale. The PIC technique uses an algorithm for particle motion based on the Newtonian laws with the time dependent equations of the continuous fluid. Crucial point of this technique is that the new momenta and energies of particles are obtained in the following timesteps from the mesh variables, and not from the previous values for the particles. A disadvantage of this method is non-central finite difference approach, which produces considerably large numerical diffusion and consequently numerical problems with a computation on a mesh. Nevertheless, this model was successfully used for supersonic flow simulations and bullet-target collisions [30].

A **Smooth Particle Hydrodynamics** (SPH) [31–34] represents another method for solution of Navier-Stokes equations. Like PIC method it is a pure Lagrangian particles method. Unlike the former one, however, it uses no underlying mesh. The absence of the mesh is compensated by the interacting particles separated by certain distances. It means that large deformations can be computed without difficulty. The foundation of SPH is the interpolation theory. Computationally, information is known only at discrete points, *i.e.* particles. The functions are evaluated using their values at the discrete points and using the interpolation kernel. Although the SPH method has been first used for astrophysical applications, the method has been recently applied to mechanical problems. The numerical difficulties are similar to those for the PIC method, *e.g.* large unphysical oscillations near shocks and non-coherency of the computational model are still present. The way to overcome them is the same for both SPH and PIC techniques. The numerical oscillations can be damped using an artificial viscosity factor. On the other hand, SPH approach is very valuable for MD technique principle foundation. It may constitute a link between pure particle oriented methods and a classical hydrodynamic approach.

3. MD and DPD programs

3.1. General characteristics

The MD program for simulations of flows of Lennard-Jones liquids in 2D systems with great numbers of particles (MDDAMP, version 2.01) was written in C language. The

program was carefully optimised with respect to CPU time and memory usage. It has several characteristic features:

1. it accepts an arbitrary number n of different types of particles, *i.e.* particles with different masses and different interaction parameters;
2. the interaction applied in our program is the short-range Lennard-Jones potential in the form:
$$U(r_{ij}) = 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right], \tag{6}$$
where ε is the well depth of the potential, σ can be roughly treated as a nearest distance of particles, and r_{ij} is the actual distance between particles i and j.
3. external gravitational force can be applied only to certain (user defined) number of kinds of particles, *e.g.* to the particles representing fluids;
4. in order to avoid growth of energy in the presence of external gravitational field, a damping coefficient, d ($0.0 \leq d \leq 1.0$), is used. In particular, we use the *leap-frog* scheme in the following form:
$$v_i^{n+1/2} = \frac{1-d}{1+d} v_i^{n-1/2} + \frac{1}{m_i(1+d)} F_i^n \cdot \Delta t, \tag{7}$$
$$r_i^{n+1} = r_i^n + v_i^{n+1/2} \Delta t, \tag{8}$$
where n is a timestep counter, Δt - the timestep. As results from (7) and (8), for $d = 0.0$ one obtains a standard version of the *leap-frog* scheme, whereas the maximum value of d ($d = 1.0$) corresponds to a complete loss of the memory of the particle velocity between two successive integration steps.

The DPD program structure is very similar to the MD one. The main differences concern the potentials. The detailed description of numerical DPD model is presented elsewhere [35].

3.2. Simulation layout and main run parameters

3.2.1. Overall system layout

The results presented below have been obtained for 2D rectangular systems consisting of two, three or four types of particles. Particles of the first kind (1), of practically infinite mass, represented unmoveable boundary layers (if present). Particles of the second kind (2) were used to construct solid granules representing porous material. The granules were built of particles much heavier than 'fluid' particles. We used the mass ratio of 10^{10} to model a rigid unmoveable granules. The set of granules occupied the lower part of the simulation box. Particles of the third kind (3) represented the liquid phase, and were placed in the upper part of the simulation box. In the MD runs the space below liquid surface between the granules was privy of any particles.

Such a system layout must be somewhat modified in the case of DPD simulations. Since in the DPD method we have only repulsive interaction, the layer of fluid quickly expands to fill the whole simulation box instead of moving down under the influence of gravitational force, maintaining constant volume. Thus, the vacuum below the fluid lower surface should be 'equipped' in positive pressure, preventing the fluid expansion. In our simulations we filled the space between the granules with light particles of fourth kind (4), characterised by the same interaction parameters as in the liquid, but having masses

10^4 times smaller. Such an 'ether' produces internal pressure that exactly equilibrates the pressure in the liquid, but its density is negligible, so the motion of the percolating fluid is practically not effected.

3.2.2. Model porous medium

Let us now give some details on the model porous medium we have used. We considered regular and irregular systems. The regular porous medium was modelled as a set of circular obstacles, distributed on quadratic network of lattice constant equal to a = 11.73 nm in the case of MD simulations and a = 362 nm in the case of DPD simulations. In another version the positions of obstacles in odd rows differed from those in even rows of $0.5a$ in the horizontal direction. The obstacle radii were chosen to be $0.1a$, $0.2a$, $0.3a$, and $0.4a$. It corresponds to the surface coverage p equal to 0.031, 0.126, 0.283, and 0.503, respectively. In our simulations, in order to study the influence of the distribution of the medium on the character of the flow we also took under consideration porous media modelled by regular systems with constant surface coverage p = 0.283 and various obstacle radii. The irregular model porous media were built of sets of non-overlapping circles distributed at random, and giving the total surface coverage p. Equal radius was assigned to all the circles.

3.2.3. Interaction and run parameters

For MD flow simulations the Lennard-Jones interaction potential was chosen. The standard argon (Ar) parametrisation has been used for the fluid, *i.e.* σ = 0.3405 nm, $\varepsilon = 1.6 \cdot 10^{-21}$ J, $m_{Ar} = 66.42262 \cdot 10^{-27}$ kg, whereas for fluid – obstacle interactions we use some arbitrary set of parameters. All simulations were performed at the temperature of $T = 100$ K in presence of external gravitational field with intensity $g = 2 \cdot 10^{12}$ m/s^2. Such a big value of the acceleration field was assumed in order to observe noticeable flow within a reasonably small number of timesteps. Equations of motion were solved with timestep Δt = 10 fs for 500 ps.

For DPD flow simulations we used a common set of potential parameters for all the interactions. After a series of tests we have chosen the following values: internal pressure equal to $1 \cdot 10^{-2}$ Pa and $\sigma = 14.4$ nm. External gravitational field with intensity $g = 1 \cdot 10^8$ m/s^2 was applied to the system. Dynamics of the system was simulated for 1500 ns with timestep Δt = 10 ps.

4. Simulation results

In two subsequent sections we discuss general qualitative (4.1), and some simple quantitative characteristics (4.2) of flows simulated within MD and DPD approaches.

4.1. Qualitative flow features

Qualitative results are shown in subsequent figures in a form of snapshots of particles' configurations. In Figure 1 we present the result of the MD simulation of the flow through regular system of obstacles. One can observe the penetration of porous medium by the liquid phase. Fluid passing layers of grains becomes more and more disintegrated (splits to separated clusters). Figure 2 shows the configuration of the system after the same time of simulation (t = 120 ps) for two different structures of the porous medium. When obstacles are positioned in columns liquid flows between them in the form of fluxes (Figure 2b), whereas in the other case (when grains in every second raw are placed between those

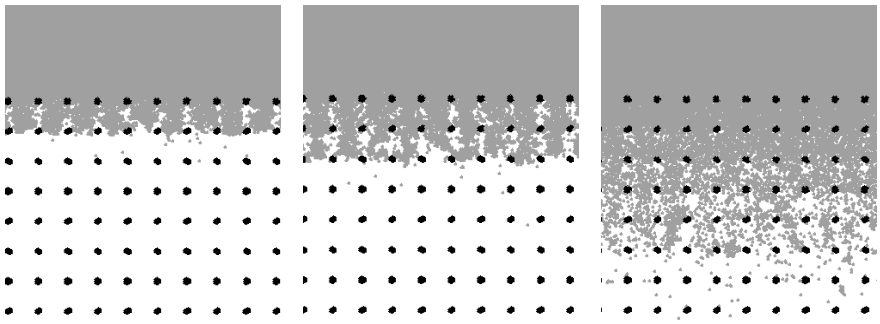

Figure 1. The flow through regular system of obstacles of the radius $r = 0.1a$ obtained in MD simulation. The particle configurations after time: (a) 60 ps, (b) 90 ps, and (c) 150 ps

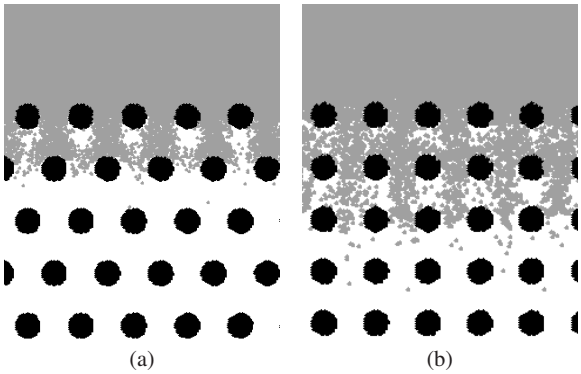

Figure 2. The configuration of the system after $t = 120$ ps for two different structures of porous medium ($p = 0.286$, $r = 4.69$ nm) (MD)

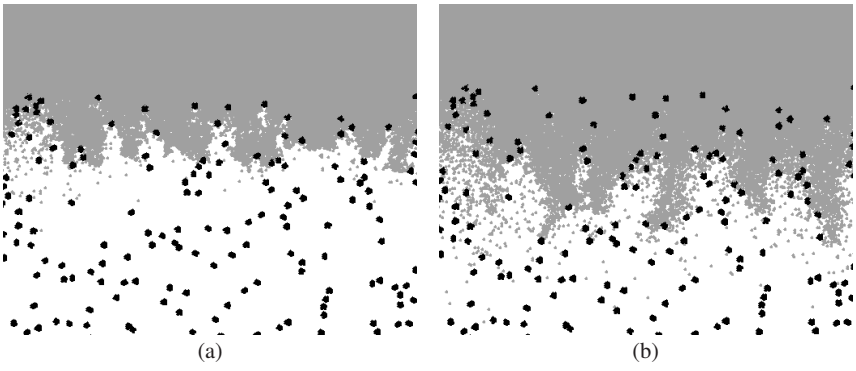

Figure 3. Flow through porous medium with randomly dispersed grains. Snapshots made after (a) 90 ps and (b) 150 ps of simulation time (MD)

above, Figure 2a) fluxes are scattered on the grains laying below and the flow is slowed down. Figure 3 presents simulated flow through porous medium modelled by randomly dispersed obstacles with the radius equal to 1.173 nm.

In order to compare the chosen simulation methods, in the following pictures we present the results of simulations performed with the aid of DPD technique. Snapshots

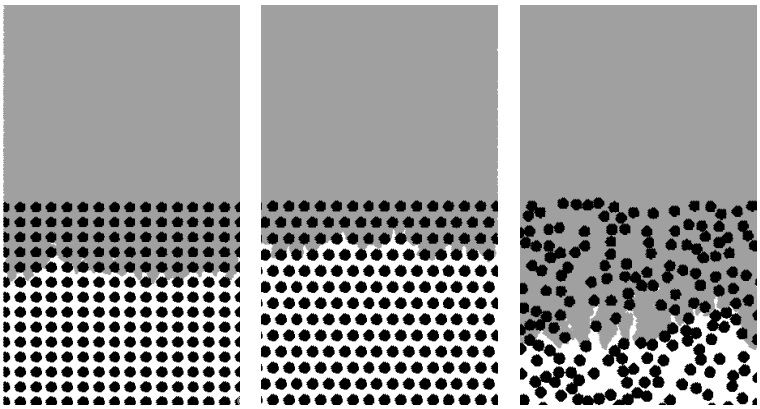

Figure 4. Results of DPD simulation of the flow through porous medium with different structures and equal grain radius: (a) $t = 130$ ns, (b) $t = 120$ ns, (c) $t = 200$ ns

of the flow through medium modelled by obstacles of radius $r = 108.6$ nm positioned in various ways are shown in Figure 4.

Compared with molecular dynamics, DPD particles form a truly mesoscopic system. Due to much softer DPD potential, the behaviour of the flow is much more liquid-like, without discontinuities seen in the MD simulations.

4.2. Quantitative features

The simulation box was divided into a number of layers (34 and 56 in MD and DPD simulations, respectively). In subsequent timesteps we calculated the concentration of fluid particles in layers. It allowed us to observe the profile of density of fluid phase along the vertical axis and how it evolves in time. In Figure 5 we present the distribution of liquid particles in several subsequent timesteps. The fluid placed initially above the porous bed by the gravitational force penetrates following layers of the medium and the accompanying wetting front moves down.

We also calculated the centroid of the liquid in subsequent timesteps. The time-dependence of the liquid centroid position enables quantitative comparison of flows through porous media with various structures. In Figure 6 we compare the liquid centroid motions for systems modelled by grains of different size placed in nodes of the same square lattice, whereas in Figure 7 we analyse the influence of the disintegration of the bed with constant surface coverage. The time derivative (the slope of the curves) estimates the velocity of the flow.

The analysis of the curves presented in Figures 6 and 7 leads to the following conclusions:

- the flow velocity for large times becomes constant in all the considered cases; this saturation is caused by the additional drag force which appears due to the interaction between the liquid and the bed particles, and compensates the gravitational force;
- for established lattice constant a (Figure 6), with the increasing radii of the grains the area within the bed available for the fluid particles decreases, and as a result the flow is slowed down;

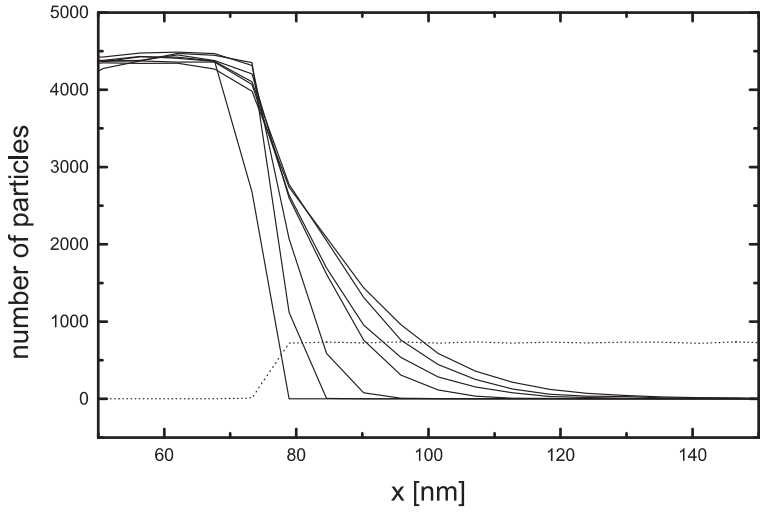

Figure 5. The plot of number of particles of liquid in following timesteps: $t = 2$, 50, 100, 200, 300, 400, 500 ps. The dotted line shows the distribution of porous bed particles. The grains were of radius $r = 1.173$ nm, and surface coverage $p = 0.286$ (MD)

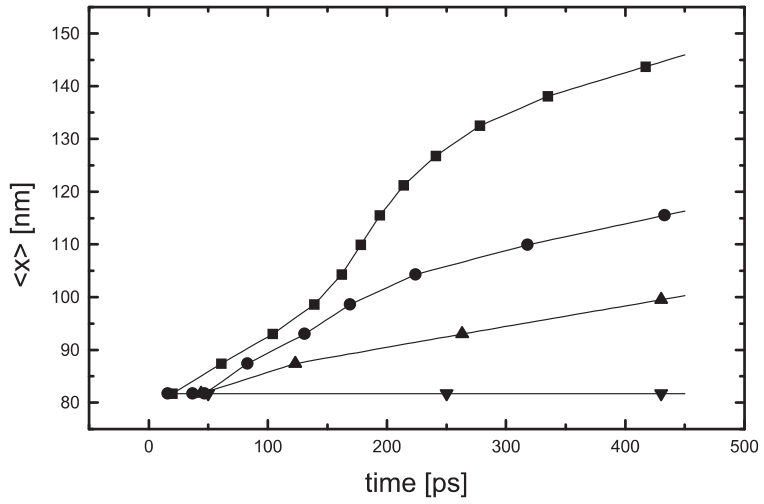

Figure 6. The plot of centre of mass position versus time for various radii of obstacles placed in the nodes of regular square lattice with the same lattice constant $a = 11.73$ nm (MD). ■ – r = 1.173 nm; ● – r = 2.346 nm; ▲ – r = 3.519 nm; ▼ – r = 4.692 nm

– for established surface coverage p (Figure 7), the centroid of the liquid moves faster for the less dispersed medium (larger r); in this case the pores in bed are larger and the percolating fluid is less dissipated.

In the same way we analysed data obtained in the DPD simulations. In Figure 8 we present the plot of centre of mass of liquid versus time which corresponds to Figure 6.

We observed similar tendencies as in MD simulations. From the slope of the curves we obtained approximate values of flow velocities for various structures of porous medium. These are presented in Table 1.

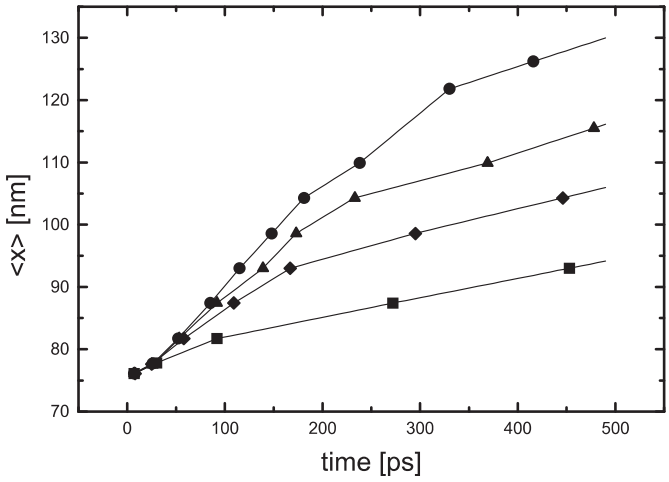

Figure 7. The plot of centre of mass position versus time for various radii of grains of porous medium with constant surface coverage $p = 0.286$ (MD). ■ – r = 1.173 nm; ◆ – r = 2.346 nm; ▲ – r = 3.519 nm; ● – r = 4.692 nm

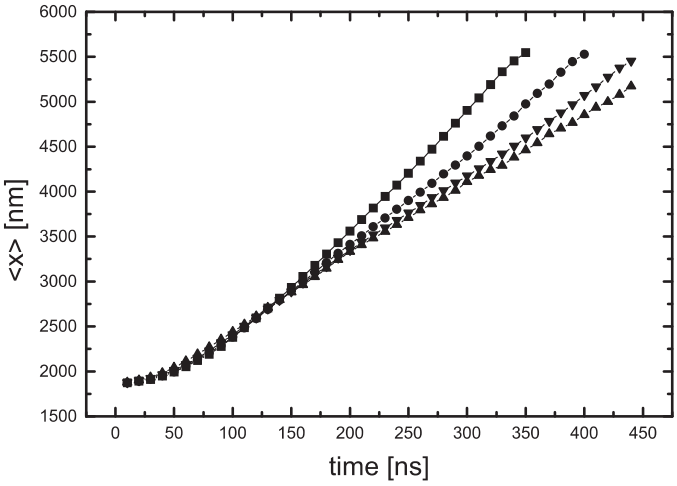

Figure 8. The plot of centre of mass position versus time for various radii of obstacles placed in the nodes of regular square lattice with the same lattice constant $a = 362$ nm (DPD). ■ – r = 36.2 nm; ● – r = 72.4 nm; ▼ – r = 108.6 nm; ▲ – r = 144.8 nm

Table 1. Values of flow velocities for percolation of fluid through beds with different radii of grains

r [nm]	v [m/s]
36.2	13.35 ± 0.09
72.4	10.53 ± 0.11
108.6	8.83 ± 0.08
144.8	7.62 ± 0.03

Comparing the flows through the beds with regularly and irregularly distributed grains of the same size we found that the structure of the porous medium doesn't influence the motion of liquid centroid.

5. Concluding remarks

An attempt to simulate the flows of 2D Lennard-Jones liquids and DPD liquids through model porous medium has been performed. Using appropriately chosen L-J potential parameters one can obtain qualitatively correct behaviour of liquid. In certain ranges of parameters the flow velocity assumes a saturated value, although the acceleration field is non-zero during the whole simulation. The saturated velocity depends in a reasonable way on the porous medium parameters. However, the fluid flow simulations realised via MD simulations demand extremely long simulation times.

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