

Charged Particle Flow Base On Mesoscale Simulation With Coupling MPCD-MD Method In Two Dimension Channel

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Abstract. Ferrofluid have magnetic behavior. In this review, has study about mesoscale colloidal system. Coupling MPCD-MD method was constructed to build a charged particle flow base on mesoscale simulation in two dimension channel. Various variation of charge and temperature to observe behavior of viscous fluid. Particle interacted with each other and external field in two dimension system. The fluid is flow in same direction in x coordinate. This simulation that was presented here covers the essential flow effect due charge and temperature in the pipe geometry. Dynamic viscosity is rising when charge. And dynamic viscosity is tend to lower value when temperature is rising.

1. Introduction

Ferrofluid are stable colloidal suspension. It consist single-domain magnetic particle coated with a surfactant in a carrier fluid. The particle has magnetic behavior. And the carrier liquid is typically an oil or water base [1].

A ferrofluid can be affected by an external force, such as magnetic field. If magnetic field has applied, it can be logic to a ferrofluid. Can control the flow of the ferrofluids. Benefit application of ferrofluid it is used in various fields, such as mechanical engineering, nuclear reactor, thermal engineering and aerospace [2–5].

In order to investigate, there is lot of design and experimentation of porous media of ferrofluid application, such as numerical experiment of ferrofluid flow phenomena in different geometries in the presence of an external magnetic field [6–15]. Strek and Jopek [15], simulated heat transfer through a ferrofluid under the influence of magnetic dipole.

Ganguly et al. [17] simulated a Two-dimensional pressure-driven flow of a magnetic fluid in a channel to investigate the influence of line source dipole magnetic field on the convective heat transfer. Youcef Amirat [18], research a differential system introduced by M.I. Shliomis to describe the motion of a ferrofluid driven by an external magnetic field. That combination of the Navier-Stokes equation.



Habib Aminfar [19], simulated the interactions of magnetic nanoparticles are based on magnetic dipole–dipole interaction potential. Simulations reveal that the system with magnetic nanoparticles agglomerates faster than that of non-magnetic nanoparticles.

P. K. Papadopoulos [20], investigate the accuracy of an analytical solution for the magnetization equation and assess its validity when used for non-uniform magnetic fields. It is found that it can be very helpful as a means of estimating the magnetization, especially for strong magnetic fields with low gradients; second, to examine the effects of the magnetic field on the flow and study the relevant importance of the magnetic terms of the momentum equation. It is revealed that the axial pressure drop depends linearly on the volumetric concentration and that the magneto viscosity effect is negligible in cases of non-uniform magnetic fields.

Many investigation of ferrofluids behavior, which are study the hydrodynamic of flow single phase model of colloid mixture and polymer-colloid mixture. Inside MPCD algorithm is a Stochastic Rotation dynamic to ensure that collision change the direction and the velocity. But MPCD algorithm come to summaries of cell average. Which mean the particle is only interacted with cell.

For solving when a single particle is experience a force with other particle or experience an interference from the outside system then we add MD method. So in this time we apply a coupling MPCD-MD in this numerical simulation. This MPCD method is adapted from [21]. In the MPCD algorithm we use to find momentum and angular momentum, however SRD unable to calculate the angular momentum. Charge fluids show that many behavior and rheological characteristics when it flowed [22].

Takehiro Yamamoto [23], create a numerical simulation of star polymer under shear flow using a coupling method of multi-particle collision dynamics and molecular dynamics. The numerical results agree well with both experimental results and predictions by other numerical methods.

2. Numerical Methods

Numerical methods in this paper we modeled a charge fluids flow under Cartesian coordinate. This fluid were represented by particle. In numerical case, MD and BD simulation was performed and studied by many researcher. Larson and Edwards [24], simulation the motion of charged fluids was modeled by MD, and the flow of fluid computed via MPCD. MPCD algorithm and MD algorithm was coupled to consider interaction of charge particle and other external field. Then the hydrodynamic interaction also considered with MPCD.

The Cartesian coordinate system was employed. The direction of flow was x and the velocity profile was $u(y)$. the system length is L_x and height is L_y , for MD and MPCD computation. The system is divided in to a small cell with length a , which is declared to be collision cells.

Assume we have system with N particle then distributed randomly into 2D channel of volume V . And particle has position and velocity \vec{r}_i, \vec{v}_i . MD is part of solving newton's Equation of motion which many particle in cell interacting with each other.

$$\vec{F}_i = m_i \frac{d^2 \vec{r}_i}{dt^2} = \partial \frac{\vec{U}(r_1, r_2, \dots, r_n)}{\partial r_i} \quad (1)$$

Where m_i is particle mass of i -th particle, r_i the particle position. Using velocity verlet method that can give the position, velocities and acceleration of particle in the system as a function of a time. In this study, we represent of ferrofluid flow as a system of a charged particles.

On the MD method, the equation for liquid particle inside a system is:

$$m_i \frac{d^2 r_{ij}}{dt^2} = \sum_{j \neq i, j=1}^N \vec{F}_{ij} + \sum_{j_w \neq i, j=1}^{N_w} \vec{F}_{ij} + \vec{F}_{ext} \quad (2)$$

Where i , j represent of particle, and \vec{i} is the unit vector in xy-coordinate. The first section of the equation is the potential force between particle i and all particle j in the cell. The last term is represents the external force, such as magnetic field and electric field.

$$\vec{F}_{ij} = k \frac{q_i q_j}{r_{ij}^2} \vec{r}_{ij} \quad (3)$$

And then to calculate potential force between particles in the cell, using coulomb equation (3) to find total force on each particle in the collision cell. That denoted by

$$\vec{F}_i = \sum_{j \neq i}^N \vec{F}_{ij} \quad (4)$$

Using velocity verlet method particle i interacted in the small cell of system to reduce amount of the total interacted particle in the system. Because the part of simulation who take lot of time is updating the velocity. Thereby array separation is made from particle data, is changed in to link cell binning [25].

In the case of external field we use the magnetic field. The direction the magnetic field is a cross product, the magnetic force on a charge q , moving with velocity in a magnetic field B is

$$\vec{F}_{mag} = q(\vec{v} \times \vec{B}) \quad (5)$$

This is known as Lorentz force law, in the presence of both electric and magnetic fields, so total force in q would be

$$\vec{F}_{ext} = q[\vec{E} + (\vec{v} \times \vec{B})] \quad (6)$$

At this simulation, the magnetic field is coming from solenoid that magnetic field has given value by B .

So equation (4) by newton 2 law of motion, become

$$\sum \vec{F} = m_i \vec{a}_i \quad (7)$$

That $\sum \vec{F}$ is come from equation 3 and 6. Thereby

$$\begin{aligned} \vec{F}_i + \vec{F}_{ext} &= m_i \vec{a}_i \\ \frac{\vec{F}_i + \vec{F}_{ext}}{m_i} &= \vec{a}_i \end{aligned} \quad (8)$$

That force change the acceleration, which correlated to each particle velocity.

3. Simulation

The fluids is represented by same charged particle with mesoscopic scale.

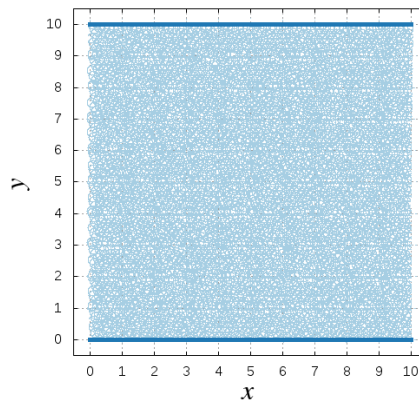


Figure. 1. Fluid in xy-coordinate, which is represented by particle.

First, the particles is interacted with other particle in cell, which is can experience a coulomb interaction with fellow. When there is an external forces, the particles interacted simultaneously with that external forces. So in this part, moving particle is calculate by Molecular Dynamic.

The motion of charge particle was computed using velocity verlet method expressed by following equation:

$$\vec{r}_i(t + \Delta t_{MD}) = \vec{r}_i(t) + t_{MD} \vec{v}_i(t) + \frac{(t_{MD})^2}{2m_i} \vec{F}_i(t) \quad (9)$$

$$\vec{v}_i(t + \Delta t_{MD}) = \vec{v}_i(t) + \frac{\Delta t_{MD}}{2m_i} [\vec{F}_i(t + \Delta t_{MD}) + \vec{F}_i(t)]$$

(10)

Where r_i , v_i and m_i are the position vector the velocity vector, and the mass of particle. Then Δt_{MD} show that the time increment in the MD simulation part. So

$$\Delta t_{MD} = \Delta t_{MPCD} / 5 \quad (11)$$

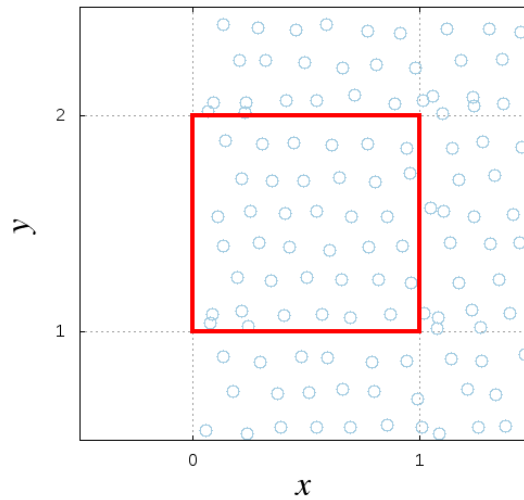


Figure. 2. Small part of system (cell), this cell refer to collision cell. The cell is divided by small red rectangle. Any particle in this cell is collide and rotate.

Then this particles is experienced collision with fellow. Not in pair, but collision occurs in a cell at once. That illustrated in fig. 2 who then experience a rotate in SRD.

In MPCD algorithm who occur SRD rotation, come into two step. The streaming step and collision step. In streaming step, particle position $\vec{r}_i(t)$ is updating base on :

$$\vec{r}_i(t + \Delta t_{MPCD}) = \vec{r}_i(t) + \vec{v}_i(t) \Delta t_{MPCD} \quad (12)$$

Which Δt_{MPCD} is time increment in MPCD algorithm. In the second part particle velocity i can be changed by a stochastic rotation matrix R_c , with angle rotation α via

$$v_i(t + \Delta t_{MPCD}) = \vec{u}_c(t) + R_c [\vec{v}_i - \vec{u}_c(t)] \quad (13)$$

Where \vec{u}_c is average velocity in cell. In the MPCD collision step show that momentum particle in the cell is redscribe.

Then we apply boundary condition in the system, invers collision in $y = 0$ and $y = H$. And continuously in $x = 0$ and $x = L$.

For computing value of dynamic viscosity and thermal conductivity is come from [26]

$$\eta = \rho k_B T \frac{1 - e^{-\rho}}{2(e^{-\rho} - 1 + \rho)} \quad (14)$$

And

$$\lambda = \rho k_B T \frac{\rho - 1 + e^{-\rho}}{1 + \rho - e^{-\rho}} \quad (15)$$

4. Results and Discussion

With consideration fluid which have charge in it, fluid representing with particle with same charge. First, we simulate with numerical for interaction charge particle who has given into fluid. At this time we investigate fluid behavior through different viscosity of fluids.

With using parameter $A_0 = 1$, $R_{SHIFT} = 0.5$, $GhostP = 0$, $N_X = 30$, $N_Y = 30$, $N_{AV} = 10$, $m = 1$, $k_B = 1$, $T = 0.4$, $Seed = 1$, $Res = 1e-4$, $Gamma = 0$, $p_I = 20$, $p_O = 10$, $k = 20$, $B = 15$.

Particle interaction with each other and external force was computed by MD algorithm. Any collision and rotation particle computed by MPCD algorithm. In this section using iteration by $t_{MPCD} = 50$, and $\Delta t_{MD} = 0.2$. We use variation charge each step is 300 coulomb differential.

This fluid was simulated in the same direction with x . And then we analyze using regression analysis. Thereby we calculate the average $f(x)$ to find dynamic viscosity in the system.

The first behavior which we investigate is behavior fluid when we give different fluid temperature at different simulation.

Fig. 3 and 4 has show that relation dynamic viscosity with temperature. Viscosity value is tended to lower value if we observing in a whole simulation. In this simulation when temperature is the free variable there are critical point. In fig. 3 has 1, and in fig. 4. has 2 critical point. In this simulation, this critical point we suppose a statistically error due unlinearity graph.

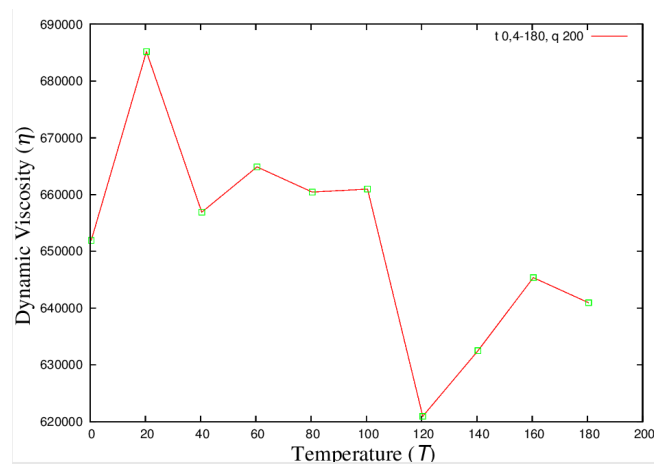


Figure. 3. Comparison of dynamic viscosity with charge function with MPCD-MD method with $q = 200$

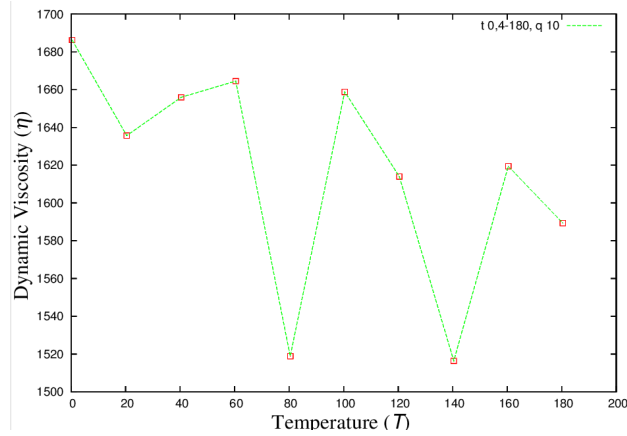


Figure. 4. Comparison of dynamic viscosity with charge function with MPCD-MD method with $q = 10$

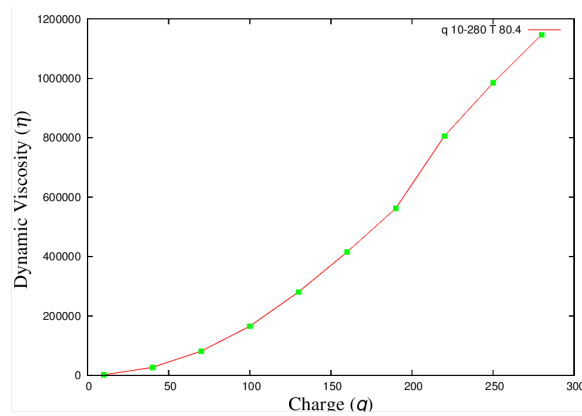


Figure. 5. Comparison of dynamic viscosity with charge function with MPCD-MD method at $T = 0.4$

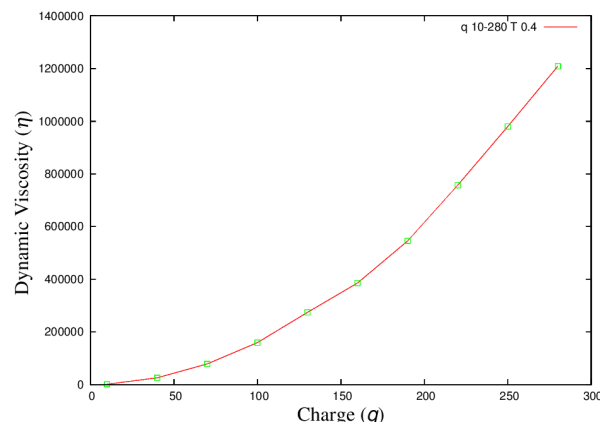


Figure. 6. Comparison of dynamic viscosity with charge function with MPCD-MD method at $T = 80.4$

Then we investigate another behavior, which is relation between charge fluid and dynamic viscosity. Using parameter $A_0 = 1$, $R_{SHIFT} = 0.5$, $GhostP = 0$, $N_X = 30$, $N_Y = 30$, $N_{AV} = 10$, $m = 1$, $k_B = 1$, $q_p = 10$, $Seed = 1$, $Res = 1e-4$, $Gamma = 0$, $p_I = 20$, $p_O = 10$, $k = 20$, $B = 15$.

Which $T_{MIN} = 0.4$ and $T_{MAX} = 80.4$. In each step same with step in previously declared which is use 50 time step in each repetition.

Fig. 5 and 6 has show that relation dynamic viscosity with charge. In this simulation we simulating fluid with charge variation. And we test with other different temperature. In this section has show that fluid viscous is rising when we add more charge in to system. This relation is show the linearity between viscosity with charge who has given in the system.

5. Conclusion

Particle base fluid flow simulation at mesoscopic scale was simulated with MPCD-MD method for charged particle. From the result was shown that dependency of viscosity with temperature is tend to lower value. In this case this fluid who have been simulated is fit to generally fluid. Another numerical result and experimental data must be proven to support this investigation. And another case is dependency fluid between viscosity and charge show that linearity relation.

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