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Numerical study of particle capture efficiency in fibrous filter

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Abstract. Numerical simulations are performed for transport and deposition of particles over a fixed obstacle in a fluid flow. The effect of particle size and Stokes number on the particle capture efficiency is investigated using two methods. The first one is one-way coupling combining Lattice Boltzmann (LB) method with Lagrangian point-like approach. The second one is two-way coupling based on the coupling between Lattice Boltzmann method and discrete element (DE) method, which consider the particle influence on the fluid. Then the single fiber collection efficiency characterized by Stokes number (St) are simulated by LB-DE methods. Results show that two-way coupling method is more appropriate in our case for particles larger than 8 μm. A good agreement has also been observed between our simulation results and existing correlations for single fiber collection efficiency. The numerical simulations presented in this work are useful to understand the particle transport and deposition and to predict the capture efficiency.

1 Introduction

Particle transport and deposition on various obstacles placed in a fluid flow are fundamental phenomena in many environmental and industrial applications such as transport in porous media, air purification, biological engineering and chemical processes. In early studies, many researchers employed theoretical analysis [1, 2], numerical simulations [3–5] and experimental measurements [6, 7] to examine particle deposition in flow over different obstacles such as cylinders, spheres or disks [8].

The main mechanisms for particle capture are Brownian diffusion, interception and inertial impaction [9]. It is possible to estimate which collection mechanism is dominant according to the following non-dimensional parameters, Peclet number, $Pe = U D_f / D$, where $D$ and $D_f$ are Brownian diffusion coefficient and fiber diameter, intercept coefficient $R = d_p / D_f$ and Stokes number $St = \rho_p d_p^2 U / (18 \mu D_f)$, in which $\rho_p$ and $d_p$ are the density and diameter of the particle respectively. $\mu$ and $U$ are fluid viscosity and mean fluid velocity. Capture efficiency corresponding to Brownian diffusion is related to $Pe$. For this case, particles diameter less than 0.01 μm with small $Pe$ number have more opportunity to be captured. Inertial impaction depends on $St$ number. High capture efficiency is also obtained for large particles (≥ 10 μm) with large $St$ number dominated by inertial impaction. However, the interception relies on intercept coefficient $R$, which is dominant for the particle in the range of 0.1-1 μm, where these other two collection mechanisms, Brownian diffusion and inertial impaction, are relatively weak [9].

The velocity and position of the solid particle rely evidently on the fluid velocity field, thus, it is essential to acquire an accurate distribution of the velocity field for the particle trajectory analysis which is appropriately described by the Lagrangian approaches. Conventional CFD model, based on the incompressible Navier-Stokes equation, combined with Lagrangian approach is usually used to simulate the fluid-solid flows within porous media such as in fibrous filters [10]. The solid particle is viewed as mass point without volume in dilute regime (point-like approach), thus the trajectory and velocity of the particle are calculated from the equation of the motion using Lagrangian approach under consideration of the different external forces such as drag force and Brownian force [9]. It is reasonable to neglect the effect of particle on the fluid when the particle-laden flows are dilute enough [11]. Obviously, point-like approach estimates roughly the actual displacement of particle within a time step. However, particle with large size can affect significantly the flow field. In this case the volume of particle and its influence on the flow field should be considered.

For particle-laden flows, the conventional numerically methods have difficulties in adaptive unstructured grids and have to adopt moving mesh for example to assure a high-resolution near the deposit when considering the particle motion. It leads to increase the computational cost. Lattice Boltzmann method (LB) demonstrated significant advantages due to easily implementing dynamic and complex boundary conditions. In the last decades LBM has gained increasing popularity for solving fluid-solid problems [12].

Here we focus on the study of particle with large size where inertial impaction and interception mechanisms are considered. The first aim of this work is to investigate
the particle capture process using a self-written code to implement the coupling of Lattice Boltzmann and Discrete element methods (LB-DE methods), which consider the influence of the particle motion on the flow field. Another aim is to analyze the effects of Stokes number on single fiber collection efficiency.

2 Study of particle deposition: comparison between one-way coupling and two-way coupling methods

In the particle-laden flow, inertial impaction is one of the major mechanisms. We show in Fig.1 the schematic of the limit trajectory of the particle and deposit on the obstacle surface. The particles released from the distance δ to the lattice axis can be trapped. Thus we define the particle capture efficiency as \( \eta = 2 \delta / D_f \).

![Figure 1. Particle trajectory and deposition on a single obstacle.](image)

The inertial effect in particle capture can be quantified by the dimensionless Stokes number \( St \) [9, 10]. In the limiting case \( St \rightarrow 0 \), the trajectories of the particles basically correspond to the fluid streamlines and almost follow them closely. Particles can only impact the surface of the obstacle when the distance from the center of particles to the boundary of the obstacle is less than or equal to the particles radius. As \( St \) continuously increases (still for low \( St \)), both inertial impaction and interception mechanism exist and dominate under certain conditions. In this case, particles follow slightly the fluid streamlines. The reason is that the inertia of particle with low \( St \) is not intense enough and interception still plays a little role. When \( St \) is sufficiently large, inertial impaction mechanism becomes more and more stronger and dominant. Particles deviate from the corresponding streamlines as they approach the obstacle and finally deposit on the surface of the obstacle. Generally speaking, the particle with large size has a larger \( St \) number (i.e., \( d_p = 10 \ \mu m \) and the inertial impaction dominates). Hence in order to reduce the effect of interception on the particle capture efficiency, we mainly study the particle with large size in this work.

2.1 One-way coupling method

The whole fluid space is computed using the LB method. After that each solid particle is injected one by one at the inlet of the domain. The initial velocity along the flow direction is set to be equal to the fluid velocity at that position. For one-way coupling method, the force of particle on fluid dynamics can be neglected if the particle volume fraction is less than \( 10^{-6} \) [11]. The solid particle is viewed as a point without volume. It is assumed that the velocity flow field remains unchanged and is not affected by the injected particles. Then particles velocities and trajectories are directly calculated by the traditional point-like approach tracing individual particle in the Lagrangian frame [13, 14]. Following Newton’s equation is applied to calculate the particle velocity and trajectory at any time.

\[
St \frac{d\vec{v}_p}{dr^*} = \vec{u}^* - \vec{u}_p
\]

\[
\frac{d\vec{x}_p}{dt^*} = \vec{u}_p
\]

where \( \vec{u}_p \) and \( \vec{u}^* \) are dimensionless velocities of particle and fluid. Using the mean inlet velocity as reference velocity, \( x^* \) and \( t^* \) are dimensionless position and time of particle. It is worth to note that solid particles are not constrained to locate only at the same lattice nodes as the fluid particles of the LBM. Velocity of fluid \( \vec{u}^* \) located at position of the solid particles is calculated using bilinear interpolation among the four closest nodes of the lattice. A fourth order Runge-Kutta (RK) has been used to numerically solve the equations (1) and (2). Then the particle capture efficiency is estimated. The result is compared with the work of Araujo et al. [10], presented in Fig.2, who used the analytical solution for the biharmonic equation \( \nabla^4 \psi = 0 \) corresponding to Stokes equation written with stream function, given by Marshall et al. [15] to obtain the velocity flow field. Then the velocities and trajectories of point-like particles are calculated with some assumptions. The influence of particle motion on the fluid field and the interaction between particles are negligible. From Fig.2 we can conclude that fluid velocity field obtained with LB method combined with bilinear interpolation is good enough to reproduce previous results presented in literature.

![Figure 2. Capture efficiency as function of the Stokes number St. The result is compared with the work of Araujo et al. [10].](image)

2.2 Two-way coupling method

Now we use a two-way coupling method (LB-DE methods) to examine the particle transport and deposition taking into account the effect of particle volume on the flow field. The fluid phase is computed using the LB method.
For DEM part, linear spring dashpot (LSD) model is used for the normal component of the contact force. An extension of the method proposed by Cundall-Strack for shear force[16]. The effect of particle volume on the flow field is due to the particle size. Hence with the purpose of investigating influence on the particle size to the capture efficiency, various simulations with different particle diameters (8 μm, 10 μm, 12 μm) have been performed. The result of particle capture efficiency is compared with the one with obtained one-way coupling method (Fig.3).

![Figure 3. Capture efficiency as function of particle diameter obtained from one-way and two-way coupling method, respectively.](image)

When the solid particle size is small ($d_p < 8 \mu m$ for our model), particle volumes have little effect on capture efficiency. However as the particle size grows, the curve of capture efficiency obtained with one-way coupling deviates from the curve obtained with two-way coupling. For $d_p \geq 10 \mu m$ the model of one-way coupling seems to be not very accurate.

### 3 Single fiber collection efficiency

The single fiber is a filtration unit, hence it is essential to investigate the single fiber collection efficiency. In this section we focus on the study of the single fiber collection efficiency with a quantity of solid particles injected ($d_p = 10 \mu m$). The two-way coupling method (LB-DE) is used, which viewed the solid particles as objects with volume. The two-dimensional computational domain is shown in Fig 4. A circular obstacle with diameter $D_f$ representing the fiber is placed at the center of a rectangular domain of width $H$ and length $L$. A periodic boundary condition is applied on the left and right side of the domain. Both the fluid and solid particles flow out from one side will enter into the domain from other side. No-slip boundary condition is used at the surface of the fiber. The constant velocity $U = 0.67m/s$ is applied at the inlet and outlet. After the flow field achieves a steady state (velocity vector is shown in Fig 4), 500 particles are injected randomly in the projected area of fiber at the inlet of computational domain. The initial velocity of the particle along y axis is assumed to be equal to fluid velocity $u_{py} = U$, while x component is equal to zero.

![Figure 4. A steady state velocity vector of flow field around a circle calculated by LB method.](image)

For initial stage of filter, the particles in the flow field are assumed to be captured once they collide on the surface of the circular fiber[17, 18]. The single fiber collection efficiency is thus defined as[19]:

$$\eta_s = N_{collect}/N_{project}$$

(3)

where the $N_{collect}$ and $N_{project}$ represent the number of solid particle collected and the number of injected particles in the projected area of fiber respectively.

Series of snapshots from one simulation of particle transport and deposition with coupled LB-DE method are shown in Fig.5. The particle volume fraction is about $10^{-3}$. It is seen that after the particles injected in the upstream of fiber, the velocity field of fluid changed remarkably which, in turn, lead to the variation of the particle velocities and trajectories.

![Figure 5. Velocity field of fluid and particles distribution for St=0.5](image)

Fiber capture efficiency is influenced significantly by the inertial parameter $St$. Among the published literatures [20, 21], a number of impaction theories and empirical expressions have been developed to predict single fiber efficiency resulting from the inertial impaction.

Schweers et al.[7] improved the approximation of formula proposed by Suneja and Lee[22] and developed following equation for single fiber efficiency:

$$\eta_s = \frac{St + 0.8 - 2.56 - \log_{10} Re - 3.2R}{10 \sqrt{St}} (1 + R)$$

(4)

where the validity range is for $1 < Re < 60$, $\eta_s > 0.05$, $R \leq 0.15$. 


Israel and Rosner[23] investigated the aerodynamic capture efficiency of non-stokesian particles and determined the following expression for $St > 0.14$:

$$
\eta_c = \left[ 1 + 1.25(St - 0.125)^{-1} - 1.4 \times 10^{-2}(St - 0.125)^{2} + 0.508 \times 10^{-4}(St - 0.125)^{3} \right]^{-1}
$$

(5)

In order to examine the effect of $St$ on the single fiber efficiency with considering large particle with volume, a comparison between the single fiber collection efficiency obtained with our LB-DE method and that obtained from the empirical relationships calculated according to Eqs (4) and (5) is made Figure 6. In our model the Reynolds number ($Re$) and intercept coefficient are $Re \approx 7$ and $R = 0.0625$, respectively. The collection efficiency is plotted as a function of the $St$ ranging from $0.5 < St < 3$. The agreement between the simulation and empirical formula Eqs (4) is observed. However with respect to the Eqs (5), there exist a little difference with our simulation result but with the same tendency.

\[Image\]

Figure 6. Comparison between single fiber collection efficiency obtained from numerically method (LB-DE) and from the empirical correlations. $Re \approx 7, R = 0.0625$.

4 Conclusions

In this paper we studied the effect of the particle size on the capture efficiency obtained with one-way coupling and two-way coupling respectively. For small particles, one-way coupling in our model is sufficient to estimate the particle transport and deposition. The capture efficiency from our simulation agrees well with the prediction of Araujo et al. However, with respect to the larger particles, two-way coupling is more accurate owing to correct consideration of the influence of particle motion on the flow field.

The single fiber collection efficiency is investigated by LB-DE methods. The particle deposition on the fiber surface is essentially characterized by the particle Stokes number as inertial impaction plays a dominant role. It is found that the rate of single fiber collection efficiency increased from rapidly to slowly with increasing Stokes number. In dilute case, good agreement with previous study of particle capture efficiency have been observed. This coupled model can also be used to study capture efficiency in relatively dense cases. Based on these simulations, the presented model offers an appealing tool for understanding the filtration process and predicting the capture efficiency.

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