Numerical research on the filter performance of PM_{2.5} on the micro-scale of fibrous assembly

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Abstract. Numerical simulation of the $PM_{2.5}$ filter phenomenon in the internal microstructures of fibrous assembly was carried out three dimensionally by discrete element method (DEM). Eulerian method and Lagrangian method were employed to deal with the gas phase and solid phase respectively. By the direct tracking of each of the aerosol particles, the collection efficiencies of $PM_{2.5}$ were calculated under different conditions. The simulation results show that the collection efficiency of $PM_{2.5}$ decreases with the increase of porosity (ϵ) and linear density (ρ), while is found no variation with the change of particle concentration and flue gas velocity.

Introduction

 $PM_{2.5}$ in the atmosphere, which is harmful to the people's health, has been drawing more and more attention. The flue gas from coal-fired power plant is one of the main sources of the $PM_{2.5}$ in the atmosphere. Some researches show that the emission amount of $PM_{2.5}$ from thermal power plants covers about 10% of total output by human activities^[1].

The bag filter technology is one of the effective ways to reduce $PM_{2.5}$ output from power plant. It is shown by laboratory tests that the capture efficiency for the bag filter could be up to $90\%^{[2]}$, but a part of the particles are emitted into the atmosphere. In order to control the $PM_{2.5}$ more effectively, finding ways to further improve the filter technology is necessary. Relevant studies have shown that fibrous assembly is an effective material to filter out $PM_{2.5}$ particles. Fibrous assembly is a kind of filter medium, and it is composed of lots of fibers which are micron-sized and randomly distributed. Studying the effects of the characteristics of the microstructure on the filter performance is of important significance to improve the collection efficiency of fibrous assembly.

At present, in the numerical simulation studies of the filter performance of fibrous media, fibrous media are simplified as regular 2-D microstructures by most researchers^[3-5].

Microstructure of fibrous assembly

Fibrous assembly is a kind of porous medium, it is composed of lots of fibers which are micron-sized and randomly distributed, and its internal microstructure is complex. At present, more and more researches have focused on the microstructure of fibrous assembly ^[6-7].



Fig.1. Different magnification images of the microscopic cross-section of fibrous assembly

Fig. 1 shows the fiber distribution image within fibrous assembly. An optical microscope was used to observe the cross section of the material so that we could have an intuitive understanding of the internal microstructure of fibrous assembly. Through the images, the random distribution of fibers can be observed clearly.

To get a better understanding of the microstructure, the images of the test samples were taken under different porosities and linear densities, which are shown on Fig.2 respectively. Through the observation and analysis of the pictures, the characteristics of the microstructures with different porosities and linear densities can be got, which can help to build the 3-D microscopic model of fibrous assembly.



(a) $\varepsilon=0.92$ (b) $\varepsilon=0.90$ (c) $\varepsilon=0.88$ Fig.2. Images of microscopic cross-section of fibrous assembly with different porosities

Model building

Fibrous assembly is a kind of loose porous media which are filled with a large number of fibers. Considering its complex internal structure, the modeling process of the microstructure of fibrous assembly is based on the stochastic algorithm. Cuboid is selected as the micro-units of our research to describe the local microstructure inside the fibrous assembly. Cylinders are used to simulate the fibers, and the diameter of cylinders represents the corresponding size of fibers. The fiber bending and deformation of fibrous assembly caused by squeezing are ignored in our model. In the process of the model building, firstly, some random points are created in each of the cubic faces by the VB programming language. Secondly, another programming language (lisp language in AutoCAD) is used to create random spatial distribution of fibers. In the same spatial area, the random 3-D microstructures with different porosities can be obtained by modifying the number and size of fibers. Fig. 3. shows a part of the microstructure of a 3-D fibrous assembly.



Fig.3. 3-D fibrous assembly model

At the end of the modeling process, the geometry output from AutoCAD is exported to Gambit software (a preprocessor for Fluent[®] code). The exact porosity of the media is calculated in Gambit and the structure is meshed for finite volume calculations conducted by the Fluent[®] code. Fig. 4 shows the comparison of the simulation model and the real microstructure of fibrous assembly. As can be seen from Fig.4, it can be realistic to build the simulation model based on the stochastic algorithm.



(a) Real microstructure in fibrous assembly (b) cross section of the fibrous assembly model Fig.4. Comparison of the microstructure

Solution

In the process of fiber filtration, Reynolds number is typically less than one. The model of a steady, laminar, incompressible flow can be used to simulate the flow in the micro channels of fibrous assembly. There is a linear relationship between the flow velocity and the pressure drop, indicating that inertial effects are negligible ^[8]. The finite element method ^[9] applied in the Fluent code is used to solve the continuity and momentum equations:

$$\frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} + \frac{\partial u}{\partial z} = 0$$
(1)

$$\frac{\partial p}{\partial x} = \mu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right)$$
(2)

$$\frac{\partial p}{\partial y} = \mu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right)$$
(3)

$$\frac{\partial p}{\partial z} = \mu \left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right)$$
(4)

The symmetric boundary conditions for the edges of the computational area are used. There are actually no symmetric surfaces in disordered fibrous microstructures, but if the sample size is large enough, the symmetric boundary conditions will not affect the simulation results, as the flows in the fibrous assembly are mainly in the lengthwise direction and transverse flows are negligible.



Fig.5. (a) An example of the meshes on one of the symmetry boundaries; (b) Fibers with the interval mesh sizes of 3 and 6

Tetrahedral/hybrid elements are used to mesh the model^[10], and meshes close to the surface of the fibers are refined. In the irregular microstructure of fibrous assembly, there are regions where the distances between fibers are very close, and the distances between fibers are relatively far from each other at some other regions. Locally thickened meshes are deployed in the narrow gaps between the fibers so as to guarantee the requirements of computational precision. Fig. 5 (a) shows a typical mesh

on one of the symmetry planes. To ensure the results presented in this paper are independent of the number of grid points, we selected one of our models and studied the effect of mesh density on the collection efficiency and pressure drop. From Fig. 5(b), different grid interval sizes on the surface of the fibers can be observed.

The effects of interval size on pressure drop are shown in Fig. 6, the results are obtained from a medium with $d_f=24.49 \ \mu$ m, SVF=8.02%. As it can be seen from Fig.6, when the interval size ranges from 3 to 8, the increase of the interval size results in a tiny fluctuation of pressure drop. However, when the interval size rises up to 8, the pressure drops dramatically. In our studies, the interval size on the cross-section of fibers was no more than 8.



Fig.6. The effects of interval size on pressure drop

Considering the complexity of the interactions between the particles, the particles and the filtering media, the particles and the gas flow in the process of particle deposition, we have made some assumptions to simplify the model:

- 1) Static electricity and gravity force of particles are negligible.
- 2) The influence of interactions between particles on the motions of the particles is ignored. If collision efficiency between particles and trapping surface is equivalent to 1, the particles will be captured once they touch the fibers.
- 3) The interaction forces between particles have little impact on particulate motion, and there is no compressible phenomenon between particles.
- 4) When aerosol particles collide with fibers, the particles will be captured as a result of the van der Waals force between the surface of the fibers and particles. The effects of other factors such as the rebound force, which may result in the escape of particles from the fibrous surface, are also ignored.

The Lagrangian method is used to track the trajectory of each particle. In this method, the force balance equation on a particle is established to obtain the particles' position in time. At the atmospheric temperature and pressure, inertial impaction can be ignored for particles at low and moderate gas velocities. Moreover, interception plays a significant role in the filtration process ^[11-12]. For a particle whose Reynolds number is smaller than unity, the dominant force acting on the particle is the air drag force exerted by the flow ^[13]:

$$\frac{dv_{ip}}{dt} + \beta(v_{ip} - v_{if}) = 0$$
(5)

Where, v_{if} and v_{ip} are the fluid and particle velocity in *x*, *y* or *z* direction. β is the Relaxation frequency of particles:

$$\beta = \frac{1}{\tau} = \frac{18\eta}{d_p^2 \rho_p C_c} \tag{6}$$

Here d_p and ρ_p are the particle diameter and density. $Cc=1+Kn_p(1.257+0.4e^{-1.1/Knp})$ is an empirical correction factor called the Cunningham slip correction factor.

In this paper, the diameters of particles that we study are under micrometer scale. Therefore, the Van der Waalswe forces should be taken into account when the particles are close to the fibers ^[14]:

$$F_{vdw}(h) = A \frac{2}{3r[((h - r_f)/r)^2 - 1]^2}$$
(7)

Where *r* is the particle diameter and r_f is the fiber diameter. *h* is the distance between the center of the sphere particle and the center line of the fiber during the trajectory tracking. *A* is called the Hamaker constant, which is equivalent to 2.0×10^{-20} J in our paper.

The particles are treated as point masses by the Standard Discrete Phase Model (DPM) in Fluent \mathbb{Q} code. In this paper, a VB program was used to simulate the motion and capture process of the particles. In the process of particle movement, the program will calculate the distances between the particle and fibers and determine whether the particles are captured.

The collection efficiency of fibrous assembly is calculated by the number of particles captured from an aerosol flow:

$$E=(N_{in}-N_{out})/N_{in}$$
(8)

Where N_{in} is the number of particles which enter the filter rod and N_{out} is the number of particles which leave it.

In order to demonstrate the validity of the model, experimental results ^[15] are available to be compared with the simulation results. The increase degree of every curve segment reflects the collection performance of the fibrous assembly with the increase of its length. If the curve tends to be steady, we can conclude that the capture effect of the fibrous assembly has reached its maximum.

Collection efficiency with different linear density

As can be seen from Fig.7, the curves acquired by numerical simulation results are consistent with the curves acquired by experimental results^[15]. For fibrous assemblies with the same porosity, with the increase of monofilament linear density, the collection efficiency of aerosol particles gradually decreases. If the fibrous assemblies are made of fibers with smaller monofilament linear density, the fibers will have bigger surface area and stronger capture ability, which results in higher collection efficiency. At the same time, fibers with smaller monofilament linear density are more evenly distributed in the fiber rod, and the distance between these fibers is closer, so aerosol particles with smaller sizes can be captured by the fiber rod. As is shown in Fig.7, of all the fibrous assemblies being tested above, the collection efficiency of the fibrous assembly with the porosity 0.88 and the linear density 0.27 is the highest.



Fig. 7. Comparison of experimental results with simulation results of the collection efficiency of fibrous assemblies with different monofilament linear densities.

Collection efficiency with different porosity

As is shown in Fig.8, it can be found that for fibrous assemblies with the same monofilament linear density, as the porosity increases, the collection efficiency decreases, and for fibrous assembly with a smaller porosity, it can be earlier for its collection efficiency to reach the maximum. The change of length has an effect on the collection efficiency too, the collection efficiency increases with the increase of the length of filter rod. Through the observation of the four pictures above, we can find that among the four pieces of the filter rods in each picture, the first piece of the filter rods can capture more particles than the other three pieces, so we can come to the conclusion that the first half of the the filter rods plays an more important role in filtering the flue gas. As can be seen from Fig.8, the

curves obtained from the simulation are higher than that from the experiments. The possible reason is that the penetration of moisture during the experiment leads to the decrease of collection efficiency. The results of numerical simulation can effectively reflect the collection character of fibrous assembly.



Fig. 8.Comparison of experimental results with simulation results of the collection efficiency of fibrous assemblies with different porosities.

Summary

A 3-D numerical simulation model of fibrous assembly is built in our study. The numerical simulation method is adopted to study the relationship between the characteristics of fibrous assembly (porosity, linear density, flue gas velocity, particle concentration) and its filter performance. The conclusions are as follows:

1) According to the comparison of numerical simulation with experiment, results show that with the increase of the linear density, the collection efficiency of fibrous assembly decreases.

2) For fibrous assembly made of monofilaments with the same linear density, as the porosity of the fibrous assembly increases, its collection efficiency decreases. Meanwhile, for fibrous assembly with a smaller porosity, it will be earlier for its collection efficiency to reach the maximum.

3) Through further numerical simulation study on the effects of particle concentrations and gas velocities, it is found that both of them have little influence on the collection efficiency of fibrous assembly.

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