Numerical Simulation of Gas-Solid Two-Phase Flow and Deposition in a Novel Carbon Nanotubes Particles Trap

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Abstract. The effects of gas-solid two-phase flow, flow velocity, model structure and temperature on deposition characteristics in Carbon nanotubes (CNTs) particles trap were simulated by Euler-Lagrangian model, adopt Realizable k-ε Model calculation of turbulent flow in trap, tracking of particle trajectories using stochastic orbital model. The simulated results are in good agreement with the experimental results, deposition of particles at orifice edge of baffle; The adhesion of particles to the wall surface is consistent with the phenomena presented by previous simulations. With the increase of temperature, the deposition rate of particles increases. The more the number of holes in baffle, the more particles are captured. At high wall temperature, the particle aggregation positions of concentric and heterocentric baffle trap are different. The deposition of the four wall particles in the concentric hole trap is obvious at the exit location, the particle deposition of heterocentric trap on baffle is obvious. For the vertical flow field, particles are preferentially deposited on the bottom baffle, and the heterocentric trap has a higher deposition rate than that of the concentric hole. The simulation reveals the difficult flow characteristics of particles in the trap, and the conclusions obtained are of great significance to improve the reliability of the design and amplification of the trap.

1. Introduction

Micro-particle traps are generally used in diesel vehicle micro-particle post-treatment purification systems, pneumatic conveying systems, and dust removal systems, which has the shape of asymmetric channel type, radial type, rotary type, disc-shaped shunt type, diaphragm type shunt type, etc. As a key component of collecting particles, it will cause blockage and erosion when its internal structural design and arrangement are unreasonable. Such phenomena, which in turn affect the transmission efficiency of the entire system. With the development of micro-nano technology, the dispersion of CNTs and the collection of the dispersed particles have become one of the hotspots of current research. Like haze aerosol particles, if the human body breathes in more CNT particles, especially single-walled CNTs, it will be harmful to human health. Then, how to use the trap to collect the dispersed carbon nanotubes is a problem that needs to be tackled at present. The essence of trap performance lies in the flow pattern
distribution of internal gas-solid two-phase. Therefore, it is necessary to study the gas-solid two-phase flow characteristics and the trapping characteristics of CNTs in the traps.

In recent years, both industrial and academic, the flow of gas-solid two-phase flow has received widespread attention from scholars at home and abroad. Huang Huibo[1] comprehensively expounded the technology and research progress of the wall-flow diesel particulate trap. Yang Hualong[2] obtained the capture process and mechanism of diesel vehicle particle trap by combining theoretical analysis, numerical calculation and experimental research. Li Zhijun[3] studied the flow field and pressure drop characteristics in the asymmetric channel of the micro-particle trap. Zuo Ziwen[4] explored the mechanism and characteristics of charged droplet trap of dust collector. Fan Wenpeng and Qi Qi[5] numerically simulated the characteristics of particle avoidance deposition in rough wall channel, and analyzed the particle deposition rate in the range of 3-40 μm and the variation of particle deposition rate at different positions in the channel. Gao Dezhen et al.[6] obtained the change of pressure drop and volume fraction of gas-solid phase in branch pipeline through simulating the pneumatic conveying process of T-shaped pipeline. Zhang Qinghong et al.[7] proposed a coupled Eulerian fluid-solid and Lagrangian discrete particle mixing method for numerical simulation of dense gas-solid fluidized beds. On the basis of flow field structure analysis, Dan Li et al.[8] proposed a dynamic cluster structure resistance coefficient model for gas-solid risers, and obtained that the inertia difference between dense and dilute phases affected the flow behavior of dynamic spatial-temporal clusters in risers. Li Chao et al.[9] simulated the residence time distribution of particles in gasifiers.

Through the above research, most of the traps used are similar to capillary pipelines, and most of them are replaced by porous media. They are not suitable for the collection or transportation system of carbon nanotube particles. Based on the above-mentioned diesel vehicle particle trap principle, this paper innovatively designed a micro-particle trap for pneumatic conveying system. The design concept is based on carbon nanotube particles trapping system. The CFD method was used to simulate the movement characteristics of CNT particles. The relationship between flow rate, number of holes, concentric holes, concentric holes and temperature and the deposition rate of CNT particles in the trap were investigated, which provided a theoretical basis for the reliability of the design and amplification of the trap.

2. Physical model

The CNTs particles trap, as shown in Figure 1, consists of several layers of horizontal trays with a plurality of sieve-like pores, called baffles. The CNTs have a low density and a light weight, which are driven by the airflow from the bottom of the baffle capture device, and sequentially pass through the baffles from the bottom to the top, and are deposited on the baffles of each layer under the action of the turbulence. It has been verified that the collection efficiency of baffle-type capture micro-particles is above 90%, which greatly improves the utilization rate of CNTs. These particles are easily suspended in the gas stream to form an aerosol, and stayed in the gas stream for a long time. As the temperature increases, the sol condenses to form a gel. Therefore, some particles in the trap are deposited on the wall under the action of turbulent diffusion, thermophoretic force, Brownian force, etc. Another part of the particles are directly entrained by the airflow at the outlet. In brief, the flow rate, the number of openings of the baffles, the concentric and heterocentric baffles and the wall temperature have an important influence on the deposition rate of the micro-particles.

Condition settings: (1) The diameter and density is the same, respectively, and particles are rigid spherical, the size of the particles is 1 um, the total number of particles is 3.7e5. (2) The inlet particles are randomly distributed. (3) The Stokes numbers of each model are consistent. (4) Consider the influence of the drag force, shear lift, virtual mass force, pressure gradient force, particles retention time, thermodynamic change of the particles, turbulent dissipation of the particles, etc. in the flow field. (5) Because of the dilute phase transmission, the force between the particles and the particles is ignored. Considering the bidirectional coupling between the particles and the fluid, the particles is placed between the wall and the baffle as a capture mode.
3. Mathematical model

For the flow in the trap, the fluid phase is continuous phase, and the particles are dispersed phase. The random trajectory model is adopted to track the movement of particles in the Lagrangian coordinate system.

3.1. Continuous phase model

In this paper, the movement rule of the gas phase using the two-way coupling Navier-Stokes equation, because each particle in the trap after impact form different sizes of turbulent vortex baffle plate, and even have a secondary reflow phenomenon, caused by particle and baffle plate turbulent flow field in the fully developed turbulence state, by using the Realizable $k-e$ turbulence model [11] and rotational flow field of complex calculation. The transport equation of turbulent kinetic energy and dissipation rate of the model [15] is:

$$
\frac{\rho}{\rho} \frac{dG_k}{dt} = \left[ \left( \rho \frac{\sigma_k}{\sigma} \right) \frac{d\varepsilon}{dt} \right] + \rho \varepsilon - \frac{\varepsilon^3}{k + \sqrt{\varepsilon \rho}} + \frac{\varepsilon}{k} C_{\rho \varepsilon} G_k
$$

Where, $G_b$ is the turbulent kinetic energy generated by the influence of buoyancy, $G_k$ is the turbulent kinetic energy generated by the average velocity gradient, $C_1 = \text{max}[0.43, \eta/(\eta + 5)], \eta = S \kappa / \varepsilon$, $\mu = \rho C_\mu k^2 / \varepsilon$, $C_\mu = (4.04 + 60.5 k U^* \cos \phi / \varepsilon)^{-1}$, $U^* = \sqrt{S_{ij} S_{ij} + \Omega_{ij} \Omega_{ij}}$, $\Omega_{ij} = \Omega_{ij} - 3 \varepsilon \omega_{ijk} \omega_k$, $\phi = \frac{1}{3} \cos^{-1} (\sqrt{6W})$, $\Omega_{ij}$ is a laminar flow of angular velocity with angular velocity $\omega_k$ under column coordinates $W = \frac{S_{ij} S_{jk} S_{ki}}{\tilde{S}}$, $S_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$, $\tilde{S} = \sqrt{S_{ij} S_{ij}}$. Model constant: $C_\rho = 1.44$, $C_\varepsilon = 1.9$, $C_{\rho \varepsilon} = 0.09$, $\sigma_k = 1.0$, $\sigma_\varepsilon = 1.2$.

3.2. Discrete phase model

The motion of particles can be obtained by solving Newton's second law, and the governing equation of single particle motion [12] is:

$$
\frac{du_p}{dt} = \frac{18\mu}{\rho_p d_p^2} C_D \text{Re} \left( u_g - u_p \right) + \frac{g_z (\rho_g - \rho_p)}{\rho_p} + F_y
$$

Figure 1. A novel CNTs particles trap structure
Where, $d_p$ is particle diameter, $C_D$ is drag force coefficient, $Re$ is relative Reynolds number, and $\rho_g$, $u_g$, $\rho_p$, $u_p$ are gas and particle density and velocity respectively. $g_z$ is the Z component of gravity acceleration. The first term on the right is the drag force term per unit mass particle. The second term is the resultant term of gravity and buoyancy. The third term is the resultant of additional forces, including virtual mass force, thermophoretic force, Brownian force and so on. Since the particle size is less than 10μm (the particle can be inhaled), the influence of various forces on the particle should be comprehensively considered[13]. In this study, additional forces are taken into account, and the order of magnitude of various forces is shown in table 1.

Particle deposition can be calculated by assuming that the particle adheres to the wall surface at one time. The calculation formula for particle deposition velocity [14] is:

$$R_d = \sum_{n=1}^{N_p} \frac{m_p}{A_{face}}$$

where: $A_{face}$ is the area of the wall computing unit, and $m_p$, $N_p$ represents particle mass and particle number, respectively.

| Table 1. The Magnitude of various forces |
|----------------------------------------|
| Names                                  | 1 μm     | 10 μm    | 100 μm   |
| Stokes resistance                      | $0.59\times10^{-12}$ | $0.15\times10^{-9}$ | $0.82\times10^{-7}$ |
| Gravity                                | $0.77\times10^{-14}$ | $0.77\times10^{-11}$ | $0.77\times10^{-8}$ |
| Saffman shift force                    | $0.26\times10^{-15}$ | $0.28\times10^{-12}$ | $0.33\times10^{-9}$ |
| Additional mass force                  | $0.53\times10^{-16}$ | $0.64\times10^{-13}$ | $0.72\times10^{-10}$ |
| Basset force                           | $0.58\times10^{-12}$ | $0.62\times10^{-10}$ | $0.76\times10^{-8}$ |

4. The grid model and boundary settings
The model is divided with the polyhedral mesh, as shown in Figure 2, the number of grids is 86450, 136030, and 226300, respectively. The grid independence test is performed on it, finally the number of grids is selected as 136,030. In this paper, only the two-phase flow of water vapor and micro-particles are considered. The particles are incident on the inlet surface at a constant speed, randomly distributed, and the inlet of the flow field is set as the speed inlet with four different flow rates, and the value is 0.1 m/s-0.4 m/s. Using a pressure outlet, the value is a negative atmospheric pressure, and the wall temperature is a variable above 80 °C. The density of water vapor varies with temperature. In the calculation process, the non-slip wall surface is adopted, and the standard wall function is adopted at the near wall surface, and the collision between the particles and the wall surface is set as adhesion. The calculation uses the finite volume method for discrete differential equations, the convection term uses the second-order upwind interpolation method, and the solver uses the pressure-coupled SIMPLE semi-implicit method.
5. Results analysis and discussion

5.1. The effect of velocity on deposition rate of particles
The comparison of particle deposition rates in concentric (small pore) and heterocentric (small pore) baffle traps under different flow rates is shown in Figure 3. At 0.1 m/s, the particle deposition rates of the two models are the same. At 0.2-0.4 m/s, the deposition rate of concentric baffle trap decreases, which compared with that of heterocentric baffle trap. The particle deposition rate of the heterocentric hole model is higher than that of the concentric. The reason is that the flow velocity is the largest at the center, and the shear stress is dominant. In addition, Cross-hole blocking effect of baffle plate allows the particles in the turbulent motion to adhere frequently on the plate, near the wall surface, due to the binding of the wall and the fluid viscosity gradually decreases, the particles velocity gradually decreases and slowly deposited on the wall. When gas flows through the small holes on baffle plates, the pressure and velocity gradient become larger, the vorticity of the small hole region increases, and the particles in the vortex core region are smashed to the periphery of the vortex structure due to the centrifugal force, as shown in Figure 4, resulting in “aggregation”, that is, the edge of the small hole is more adhered, as shown in Figure 5, the simulation analysis results have been demonstrated by the experiment of the small trap designed by Zhu Shengkun[10].

Figure 3. Deposition rate of particles in concentric (few holes) and Heterocentric (few holes) trap
Figure 4. Eddy volume diagram of baffle (the upper is concentric and the lower is heterocentric)

Figure 5. Particle adhesion baffle orifice edge diagram

5.2. The effect of the number of holes on the particle deposition rate (e.g., heterocentric baffle)

The effect of the number of holes on the deposition rate of particles is shown in Figure 6. As the number of holes increases, the deposition rate of the particles increases, which is verified by the "preferential aggregation" effect of the vortex structure. Since more particles are deposited around the hole (experimental has been verified), as shown in Figure 7, the more the number of holes, the more obvious the "aggregation" effect and the better the adhesion. In the core area of the turbulent flow, the diffusion of the particles in the direction of the inlet and outlet is more obvious, as shown in Figure 8.
Figure 6. Particle deposition rate of baffle trappers with different number of holes

Figure 7. Particle deposition of heterocentric porous baffles

Figure 8. Particle velocity of heterocentric porous baffles
The vorticity diagram of the particles at 2s, as shown in Figure 9 and Figure 10, on the central section of the trap, the number of holes, the flow field, the vorticity structure is all symmetrical, and the "concentration" effect of the particles is also symmetry. With the combination, destruction and reorganization of the vorticity, the pulsation intensity of the vorticity changes continuously, and the flow of the particles is also constantly changing. The diffusion distribution of the particles shows the quasi-ordered structure of the flow field, which forms a nearly uniform flow vorticity with the flow field. The quasi-sequence distribution plays a role in tracking particles.

![Figure 9. Heterocentric porous baffle particles vorticity at 2 s](image)

5.3. The effect of wall temperature on the particle deposition rate

As shown in Fig. 11, the trap with a higher wall temperature is more conducive to the adhesion of the particles on the wall surface. The minimum value of the deposition rate of the higher temperature model and the maximum value of the lower wall temperature are small, and the effect of the particles adhering to the wall is the best at 0.4m/s (shown by the red dot in Figure 11). As the temperature increases, the flow velocity of the flow field increases, the turbulent pulsation of the particles becomes stronger and stronger, and the diffusion behavior of the particles becomes more obvious. The turbulent pulsation is strongest in the central region of the trap, and the flowability of the particles is strong. The field flows quickly through the baffle holes together. Due to the strong adhesion of the micro-particles, the number of stokes is small, and adheres well around to its surroundings. The particles from the inlet are deposited...
at the corners, and the particles at the outlet adhere more to the four walls. The bottom baffle (near the inlet) has the largest number of adhering particles, it is only a qualitative analysis of the collector deposition rate as shown in Figure 13. Liu Hongtao [13] elaborated the relationship between the particle deposition rate of the vertical wall of the rectangular tube and the particle flow velocity in his doctoral thesis is shown in Figure 12, and the deposition rate of the particles is comprehensively analyzed. The results show that the lower deposition rate of wall surface in the tube is higher than that of the vertical wall surface. Therefore, the results of the trap analysis of qualitative research in this study are consistent with the results of the results of the straight tube research conducted by Dr. Liu.

**Figure 11.** Wall temperature effects on particle deposition in trap

**Figure 12.** The relationship between particle deposition rate and particle velocity on the wall of straight square tube
5.4. Effect of concentric, heterocentric baffle on particle deposition rate (high wall temperature)

In Figure 14, it can be seen that the heterocentric porous baffle has a higher deposition rate of the particles, and at the inlet flow rate of 0.4 m/s, the deposition rate of the particles is the largest, and the particles flow out quickly through the holes, and the time of particles staying in the central portion of the trap is the shortest, as shown in Figure 15 and Figure 16. However, most of the particles are forced to stay at the wall of the trap and at the edge of the holes due to the interaction of various forces in the flow field.

Figure 14. Grain deposition rate curve of concentric and heterocentric baffles at high wall temperature
6. Conclusion

Through the numerical simulation of the motion characteristics of CNTs particles in the new trap, the particles deposition rates in different speeds, holes, concentric and heterocentric baffles and wall temperatures were calculated. The calculation results are in agreement with the experimental and previous research results, and the following conclusions are obtained:

(1) The inlet flow rate has an effect on the deposition rate of the particles. The deposition rate of the particles in the concentric baffle trap is symmetrically distributed with that in the concentric baffle trap. Within the studied range, the particles deposition rate in the heterocentric model is higher than that in the concentric model.

(2) The number of particle-adhering walls increases with the number of openings. This phenomenon is verified by the “preferential aggregation” effect of the vortex structure, the number of holes and the vorticity structure is symmetrical and the particles deposition position is symmetrical, respectively.

(3) The deposition rate of particles increases with the increase of wall temperature. Under the same premise, the larger the flow rate, the more the number of particles adhering to the wall, and the higher the deposition rate.

(4) Regardless of the calculation conditions, the particles are uniformly deposited on the edge of the baffle hole, which is consistent with the experiment. The particles at the inlet are deposited at the corners,
and the particles at the outlet are more adhered to the four walls, the particle deposition on the baffle plate at the exit is the most, which is consistent with the previous numerical simulation results.

(5) The above research has found out the flow law and characteristics of CNTs particles in the trap, which provides a theoretical basis for the design and scale-up reliability of the trap.

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