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This study aims at numerical simulation of nanoparticle transport in flue-gas treatment at a waste incineration plant. The purpose of this work is to assess the effect of temperature, particle size, and fluid velocity on nanoparticle transport around a single spherical collector considered as a filter medium for nanoparticles filtration. Thus, the stochastic Langevin equation was used to describe the dynamic behavior of particles with account for different forces acting simultaneously on these particles, namely, drag force, gravitational force, and Brownian force. The results indicated, on the one hand, that the effect of temperature on the nanoparticle movement increases with temperature and, on the other hand, that the fluctuation of the particle trajectory is a significant factor in decreasing the particle diameter. Concerning the effect of the fluid velocity, the role of the nanoparticles trajectory becomes more significant the higher the value of the fluid velocity. The results of this work which are expressed as the bivariate velocity and displacement distribution function aim at understanding the experimental filtration efficiency studied in laboratory conditions at two different temperatures and fluid velocities.

KEY WORDS: *numerical simulation, nanoparticles transport, trajectory analysis, Brownian dynamics, Langevin equation*

1. INTRODUCTION

Currently, bag filters are commonly used for industrial flue-gas treatment. They are considered as an efficient means of gas/particle separation. The principle of filtration is simple: the fibers composing the filter medium retain the dust particles and are regularly cleaned with compressed air. The filtration efficiency is important in industrial flue-gas treatment if the emission standards are complied with. Thus, numerous exper-

NOMENCLATURE

$\vec{A}(t)$	random acceleration, N	**Greek symbols**	
Cu	slip correction factor		
d_f	fiber diameter, μm	ε	porosity of the medium
e	radius of fluid envelope, μm	Δt	time step, s
$\vec{F}_d$	drag force, N	μ	dynamic viscosity of gas, g/cm·s
$\vec{F}_{ext}$	external force, N	ν_0'	Guasian random variable
$\vec{F}_r$	random force, N	ρ_p, ρ	particle and gas density, g/cm^3
g	gravitational acceleration, m/s^2	τ	relaxation time of particle, s
k	Boltzman constant, m^2·kg·s^{-2}·K^{-1}	τ_b	time step between successive collisions of particle, s
m_p	particle mass, kg		
T	fluid temperature, ^{o}C	τ_F	time step leading to an appreciable change in particle displacement, s
V_f	fluid velocity, cm/s		
z	distributed random numbers		

iments and numerical studies have been done with a purpose to assess the collection of particles by filtering media.

There are different approaches used for estimating the particle behavior around the collector surface by making the trajectory analysis of particles, namely, the so-called Brownian dynamics (BD). This approach has been used by several authors for estimating the particle deposition, especially by Gupta and Peters (1984), Ramarao et al. (1993), Chang and Whang (1997), Oh et al. (2002), Lantermann and Hänel (2005), and Sztuk et al. (2012). It is considered as a simplified version of the Langevin dynamics, and it has the advantage of being conceptually simple. The Brownian dynamic approach can be applied if all forces acting on particles are deterministic. Furthermore, the Brownian force should not exhibit a significant effect on the nanoparticles movement; on the other hand, the inertial impact should not be negligible.

In this study, three forces acting on particles are taken into account: drag force, gravitational force, and Brownian force. The range of particles studied in this paper is between 10 and 100 nm.

The bag filter process was studied experimentally on a laboratory scale for two operating conditions: temperature and relative humidity (RH) encountered in realistic conditions upstream of bag filters, i.e., 150^{o}C and 3% RH, and ambient temperature and humidity in laboratory conditions, i.e., 24^{o}C and 47% RH. The particles used represented the particulate mass resulting from the incineration of industrial waste containing nanomaterials. The operating conditions used in this numerical simulation corresponded to the experimental conditions in order to make comparison between numerical and experimental results, especially for T = 24°C — V_f = 1.4 cm/s and T = 150°C — V_f = 2.5 cm/s.

2. SIMULATION METHOD

The trajectory of particles moving in a gas is described by Lagrangian integration of the Langevin equation (Langevin, 1908). Thus, all forces that could affect the particles path are considered, especially the drag force, gravitational force, and Brownian force. In contrast, the effect of particle interaction is neglected by considering a dilute particle concentration and that the particles are spherical. The description of the particle path is made in this study similarly to Gupta et al. (1984).

The trajectory of nanoparticles under the action of random and deterministic forces are determined by

$$\begin{cases} \dfrac{dX_p(t)}{dt} = v_p(t) \\ \dfrac{d\vec{v}_p}{dt} = \dfrac{\vec{F}_d}{m_p} + \dfrac{\vec{F}_g}{m_p} + \dfrac{\vec{F}_b}{m_p} \end{cases}, \tag{1}$$

where F_d is the drag force. It refers to the forces acting opposite to the relative motion of particles moving with respect to the surrounding fluid. It is the fluid resistance which is proportional to the difference between the fluid velocity u and particles velocity v; F_d can be expressed as

$$\vec{F}_d = m\beta(\vec{u} - \vec{v}) , \tag{2}$$

where β is the friction coefficient related to the particle mass m_p. The quantity β is determined from the Stokes' law and expressed as

$$\beta = \frac{6\pi\mu r_p}{C_u m_p} , \tag{3}$$

where μ is the dynamic viscosity of the gas and C_u is the slip correction factor (Millikan, 1923).

The quantity F_g is the gravitational force. It is the force responsible for the particle sedimentation. The effect increases with the particle size; it can be expressed as (Xuan et al., 2004)

$$\vec{F}_g = -\frac{\pi}{6} d_p^3(\rho_p - \rho)\vec{g} , \tag{4}$$

where ρ_p and ρ are the particle and gas density, respectively, and g is the gravitational acceleration.

The Brownian force $\vec{F}_b$, resulting from random motion, is the product of the particle mass and random acceleration, $A(t)$, that depends only on time and represents the Gaussian white noise process in stochastic terms. The effect of Brownian force increases with decrease in the particle size. It is assumed to be random in direction. This force can be expressed as

$$\vec{F}_\mathrm{b} = m_\mathrm{p}\vec{A}(t)\,. \tag{5}$$

With account for Eqs. (2), (4), and (5), Eq. (1) may be rewritten as

$$\begin{cases} \dfrac{dX_p(t)}{dt} = v_p(t) \\ \dfrac{dv}{dt} = \beta\left(u - v(t)\right) - g\left(1 - \dfrac{\rho_\mathrm{g}}{\rho_\mathrm{p}}\right) + A(t) \end{cases}. \tag{6}$$

The system can be solved analytically as described by Lantermann et al. (2007)

$$v(t) = v(t_0)e^{-\beta\Delta t}) + (1 - e^{-\beta\Delta t})\left(u + \frac{F_\mathrm{ext}}{m_\mathrm{p}\beta}\right) + \int_{t_0}^{t} e^{-\beta\Delta t}A(t)dT\,, \tag{7}$$

$$x(t) = x(t_0) + \frac{v(t_0)}{\beta}(1 - e^{-\beta\Delta t}) + \left(\Delta t - \frac{1}{\beta}(1 - e^{-\beta\Delta t})\right)\left(u + \frac{F_\mathrm{ext}}{m_\mathrm{p}\beta}\right) + \frac{1}{\beta}\int_{t_0}^{t}(1 - e^{-\beta\Delta t})A(t)dT, \tag{8}$$

where F_ext is the external force, including gravitational force, and $\Delta t = t - t_0$ is the time step.

In order to calculate the integration of the system, the time step should be sufficiently small which enables one to consider the fluid velocity and the influence of external force to be constant during the time step. Consequently, Δt should be of order of the relaxation time of particles $\tau = \beta^{-1}$, and

$$\tau_\mathrm{b} < \Delta t < \tau_\mathrm{F}\,,$$

where τ_b is the time step between successive collisions of the particles surrounding the fluid molecules, τ_F is the time step which could lead to an appreciable change in the particle displacement due to the interaction forces that are considered negligible in this study.

As the random acceleration $A(t)$ represents a stochastic process, the bivariate distribution function has been used to calculate the integration similarly to Chandrasekhar (1943) and developed by Ramarao et al. (1993) and Ermak and Buckholz (1994).

2.1 Initial Condition of Particles Position

In the Cartesian coordinates, the movement of particles is studied within a control cell which is considered as a basic unit including a single fiber. This is surrounded later by a fluid envelope of radius e which is determined as follows:

$$e = \frac{d_f}{2\sqrt{1-\varepsilon}}, \tag{9}$$

where d_f is the fiber diameter and ε is the porosity of the medium.

The fluid flow, which is the carrier phase, is two-dimensional. Furthermore, the initial position of the entering particles is located at $x = -e$ and the abscissa extends from $y = 0$ to $y = e$. For a more general case

$$y = ze, \tag{10}$$

where z denotes the distributed random numbers $0 \le z \le 1$.

On the other hand, the initial particle velocity is determined analytically similarly to (Shapiro and Zarutskaya, 2000) as a normal distribution:

$$\nu = u(r_0) + \nu_0', \tag{11}$$

where ν_0' is the Gaussian random variable with the following properties:

$$\langle \nu_0' \rangle = 0, \quad \langle \nu_0' \nu_0' \rangle = \frac{2KT}{m_p},$$

where K is the Boltzmann constant.

3. RESULTS

Simulations were carried out for studying trajectory of the particles of diameter 30 nm in two different operating conditions: temperature and fl uid velocity encountered in realistic conditions upstream of bag fi lters, i.e., 150°C and V_f = 2.5 cm/s and ambient temperature in laboratory conditions, i.e., 24°C with V_f = 1.4 cm/s.

The simulation of the particle displacement equation which is applied at some initial position indicates that the effect of temperature on the particle motion at 150°C is more signifi cant than at 24°C. Indeed, there is an important fl uctuation in the particle trajectory at 150°C. Vertically, the movement of particles changes in the range of 10 μm, while the fi ber diameter is 20 μm, hence, the probability that the particle contacts the fi ber surface is higher at 150°C than at 24°C. This result is in agreement with the result of Peukert and Loffler (1991) who demonstrated experimentally that the collection of nanoparticles by a fi lter becomes more effective with increasing temperature.

In order to evaluate the particle collision velocity on the fiber surface, which could lead to a potential particle rebound, the velocity of particles of size 30 nm was

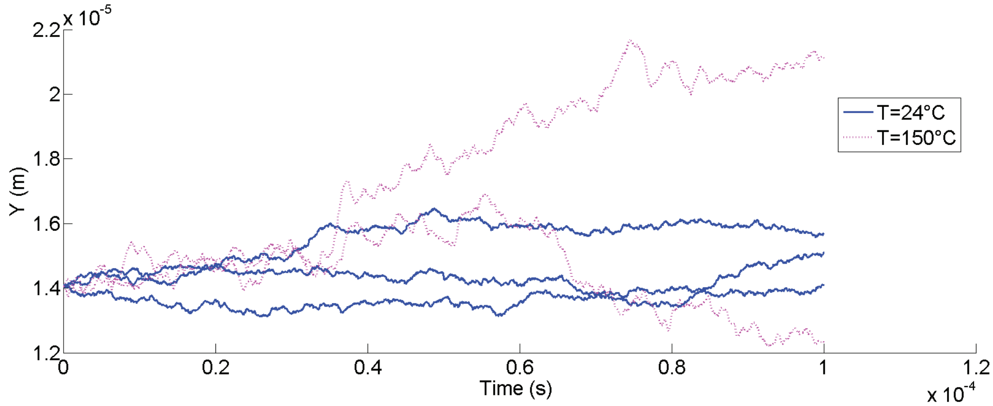

FIG. 1: Trajectory of particles 30 nm in size at T = 150°C — V_f = 2.5 cm/s and T = 24°C — V_f = 1.4 cm/s

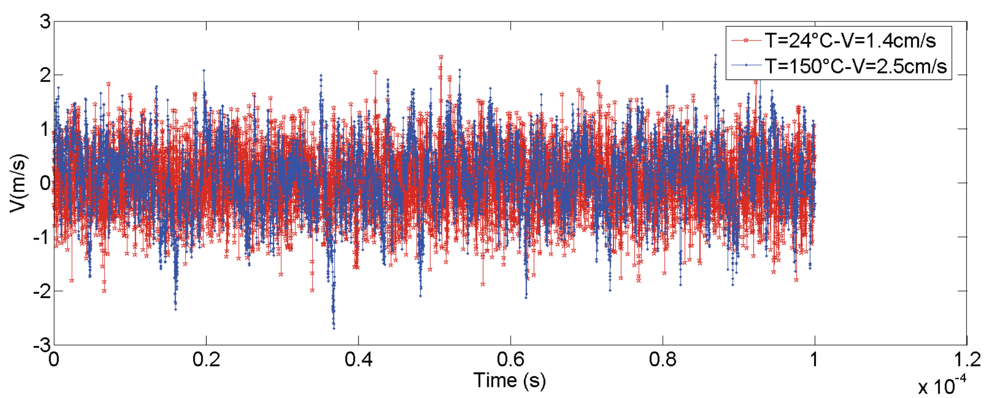

FIG. 2: Velocity of particles 30 nm size at T = 150°C — V_f = 2.5 cm/s and T = 24°C — V_f = 1.4 cm/s

calculated for two different operating conditions: T = 150°C — V_f = 2.5 cm/s and T = 24°C — V_f = 1.4 cm/s. The results of Fig. 2 show that there is no significant difference in the velocity between the two operating conditions; in other words, the collision velocity of particle on the fiber surface is the same at a temperature of 150°C and of 24°C. According to the simulation results of Scheibel**[Q3]** and Porstendörfer (2005), there is no thermal rebound for nanoparticles of size 3.5–130 nm. Hence, the capture probability of a particle by the fiber surface is the same at 150°C and 24°C.

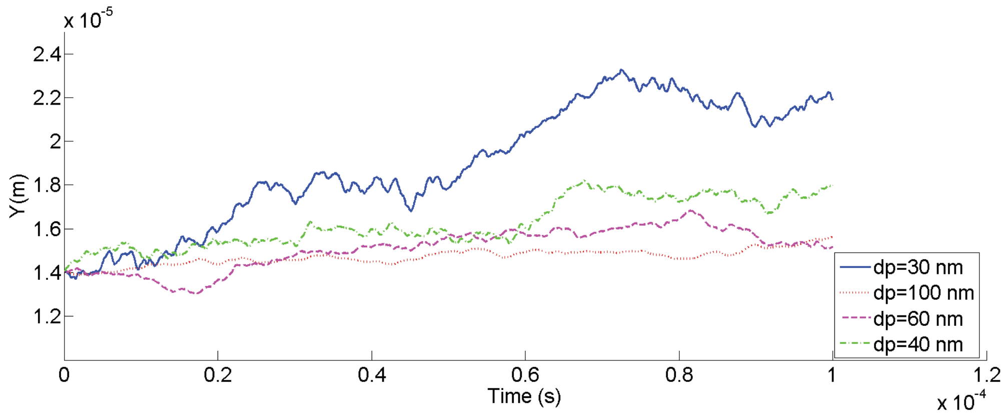

FIG. 3: Trajectory of particles with d_p = 30 nm, d_p = 40 nm, d_p = 60 nm, and d_p = 100 nm at T = 150°C — V_f = 2.5 cm/s

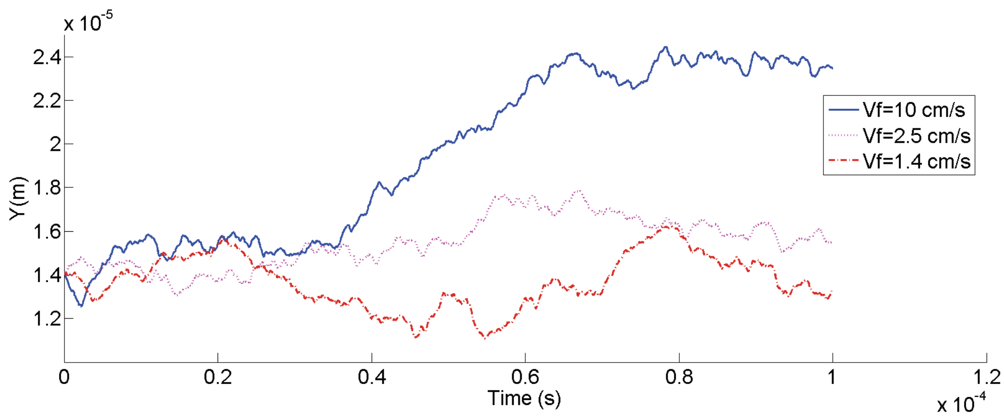

FIG. 4: Trajectory of particles with d_p = 30 nm at T = 150°C

Furthermore, the study of the particles size effect on the particle trajectory is important. The motion of particles was calculated for four different particle diameters at the same temperature and fl uid velocity; Fig. 3 indicates clearly that the fluctuations of the particle trajectory increase with decreasing of particle diameter.

Figure 4 compares the vertical displacement of particles of 30 nm in diameter at different fluid velocities and T = 150°C. The results show that the influence of fluid velocity variation is negligible for V_f = 1.4 cm/s and V_f = 2.5 cm/s. In contrast, the effect becomes important for thefluidvelocityequalto10cm/s.

4. CONCLUSIONS

The paper presents a numerical simulation developed for studying nanoparticle transport within a gas. The simulation of nanoparticles movement is studied around a filter fiber within a control cell which is considered as the basic unit. The results show the notable effect of operating parameters of gas on the particle trajectory, especially particle size and fluid temperature. The effect of temperature on the particle movement increases with temperature. Indeed, the vertical fluctuation of the particle trajectory around the filter fiber at 150^{o}C is in a range of 10 μm, while at a lower temperature of 24^{o}C, the particle fluctuates in a range of 3 μm. This result indicates that at a higher temperature, the probability of nanoparticle collection by the fiber in the control cell is higher than at a lower temperature. On the other hand, the study shows that the particle size has a significant effect on the particle trajectory so that the motion of small particles is more important than of larger ones. In contrast, the fluid velocity effect is negligible in comparison with the case at V_f = 1.4 cm/s and V_f = 2.5 cm/s.

The present numerical simulation offers an efficient way of explaining the experimental results obtained by us on a laboratory scale, particularly, the filtration efficiency of a down-size bag-filter operating at temperature and relative humidity encountered in realistic conditions upstream of bag filters, i.e., 150^{o}C and 3% RH, and at ambient temperature and humidity in laboratory conditions, i.e., 24^{o}C and 47% RH.

REFERENCES

Chandrasekhar, S., Stochastic problems in physics and astronomy, *Rev. Mod. Phys.*, vol. **15**, no. 1, pp. 1–89, 1943.

Chang, Y.-I. and Whang, J.-J., Particle deposition behavior simulated by the stochastic method, *J. Petrol. Sci. Eng.*, vol. **22**, no. 1, pp. 189–203, 1999.

Ermak, D. L. and Buckholz, H., Numerical integration of the Langevin equation: Monte Carlo simulation, *J. Comp. Phys.*, vol. **35**, no. 2, pp. 169–l82, 1994.

Gupta, D. and Peters, M. H., A Brownian dynamics simulation of aerosol deposition onto spherical collectors, *J. Colloid Interface Sci.*, vol. **104**, no. 2, pp. 375–389, 1984.

Langevin, P., On the theory of Brownian motion, *Am. J. Phys.*, vol. **65**, no. 11, pp. 1079–1081, 1997.

Lantermann, U. and Hänel, D., Particle Monte Carlo and lattice-Boltzmann methods for simulations of gas–particle flows, *Computers & Fluids*, vol. **36**, no. 2, pp. 407–422, 2007.

Millikan, R. A., Relative motion between the particle and flow, *Phys. Rev.*, vol. **22**, pp. 1–40, 1923.

Oh, Y.-W., Jeon, K.-J., Jung, A.-I., and Jung, Y.-W., A simulation study on the collection of submicron particles in a unipolar charged fiber, *Aerosol Sci. Technol.*, vol. **36**, no. 5, pp. 573–582, 2002.

Peukert, W. and Loffler, F., Influence of temperature on particle separation in granular bed filters, *Powder Technol.*, vol. 68, pp. 263–270, 1991.

Ramarao, B. V., Tien, C., and Mohan, S., Calculation of single fiber efficiencies for interception and impaction with superposed Brownian motion, *J. Aerosol Sci.*, vol. **25**, no. 2, pp. 295–313, 1994.

Scheibel, H. G. and Porstendorfer, J., Penetration measurements for tube and screen-type diffusion batteries in the ultrafine particle size range, *J. Aerosol Sci.*, vol. **15**, no. 6, pp. 673–582, 1984.

Shapiro, M. and Zarutskaya, T., Capture of nanoparticles by magnetic filters, *J. Aerosol Sci*., vol. **31**, pp. 907–921, 2000.

Sztuk, E., Przekop, R., and Gradoń, L., Brownian dynamics for calculation of the single fiber deposition efficiency of submicron particles, *Chem. Process Eng*., vol. **33**, no. 2, pp. 279–290, 2012.

Xuan, Y. and Yao, Z., Lattice Boltzmann model for nanofluids, *Heat Mass Transfer*, vol. **41**, pp. 199–205, 2004.