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# Influence of pipe length and flow rate on nano-particle deposition in laminar circular pipe flows

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**Abstract**
The Lagrangian particle tracking provides an effective method for simulating the deposition of nano-particles as well as micro-particles as it accounts for the particle inertia effect as well as the Brownian excitation. However, using the Lagrangian approach for simulating ultrafine particles has been limited due to computational cost and numerical difficulties. The aim of this paper is to study the deposition of nano-particles in cylindrical tubes under laminar condition using the Lagrangian particle tracking method. The commercial Fluent software is used to simulate the fluid flow in the pipes and to study the deposition and dispersion of nano-particles. Different particle diameters as well as different pipe lengths and flow rates are examined. The results show good agreement between the calculated deposition efficiency and different analytic correlations in the literature. Furthermore, for the nano-particles with higher diameters and when the effect of inertia has a higher importance, the calculated deposition efficiency by the Lagrangian method is less than the analytic correlations based on Eulerian method due to statistical error or the inertia effect.


**Keywords:** Nano-particle deposition; Lagrangian particle tracking method; Laminar flow; Fully developed flow; Pipes; Fluent software.

## 1. Introduction
Aerosol deposition in cylindrical tubes is a subject of interest to researchers and engineers in many applications of aerosol physics and metrology. Investigation of nano-particles in different aspects such as lungs, upper airways, batteries and vehicle exhaust gases is vital due the smaller size, adverse health effect and higher trouble for trapping than the micro-particles. For example, most particles larger than 5μm are deposited in the nose and upper respiratory walls; however, smaller particles including some nano-particles can pass into the lung airways and compromise human health [1]. Furthermore, studies on deposition efficiency in lungs, upper airways, batteries and vehicle exhaust gases are some examples of particle deposition in cylindrical tubes.

In the literature, numerous studies have developed theoretical expressions for particle deposition in smooth tubes in laminar flow regime. Thomas in 1967 [2] developed an analytical expression for a large range of particle diameters. Ingham, in 1975 and 1991, developed a model for calculating the deposition efficiency in a fully developed flow in a cylindrical tube and in the entrance region of a cylindrical tube [3, 4]. For laminar parabolic flow conditions, Yeh and Schum in 1980 [5] derived an analytical equation to calculate the deposition of particles. Cohen and Asgharian in 1990 developed an empirical expression for the deposition efficiency of particles larger than 10nm [6]. Most of these studies have used the mass diffusion equation for the concentration of particles to find an analytic correlation for the deposition efficiency. Therefore, these models often ignore particle inertia effect for aerosols smaller than 200 nm. In the absence of inertial effects, an efficient Eulerian diffusion model that treats the particle phase as a dilute chemical species can be used [7]. However, the effects of inertia for aerosols for fine particles have not been fully quantified [7]. Lagrangian particle tracking may provide an effective method for simulating the deposition of macro- and nano-particles, which can account particle inertia effect. Furthermore, the Lagrangian approach has the ability to include the effect of additional body forces that may be action on each individual particle [7, 8].

In this study, a Lagrangian particle tracking method is used to calculate the deposition of nano-particles in cylindrical tubes under the fully developed laminar flow regime. The deposition efficiency is calculated for different flow rates, various tube lengths and different particle diameters, and the results are compared with the earlier analytical correlations.

## 2. Mathematical modelling

In this paper, the commercial Ansys-Fluent software is used for solving the governing equations of fluid flow and particle equation of motion. The steady-state continuity and momentum equations for the gas phase (air) are first solved using the simple method. Then, one-way coupled trajectories of mono-dispersed submicron particles ranging in diameter from 5 nm to 100 nm are calculated based on the Lagrangian method by integrating the particle equation of motion. In this range of particle diameters, dispersion of nano-particles is mainly attributed to the Brownian force; therefore, the appropriate equations for spherical particle motion expressed as [9, 10]:

$$\frac{du_i^p}{dt} = \frac{18\mu}{d_p^2 \rho_p C_c}(u_i^g - u_i^p) + F_{Brownian} \tag{1}$$

Here $u_i^p$ and $u_i^g$ are, respectively, the components of the particle and local fluid velocity, $\mu$ is the fluid viscosity and $\rho_p$ is the particle density. In Equation (1), $C_c$ is the Cunningham correction factor to the Stokes drag law, which is given as [11-13]:

$$C_c = 1 + \frac{2\lambda}{d_p}(1.257 + 0.4e^{-(1.1d_p/2\lambda)}) \tag{2}$$

where $\lambda$ is the mean free path of air, which is equal to 65nm.

The Brownian force is modelled as a white noise process [14]. Accordingly, the amplitude is given as:

$$F_{Brownian} = \zeta\sqrt{\frac{\pi S_0}{\Delta t}} \tag{3}$$

where $\zeta$ is a zero-mean, unit-variance independent Gaussian random number, $\Delta t$ is the time-step for particle integration and $S_0$ is a spectral intensity function defined as [15]:

$$S_0 = \frac{216\nu k_B T}{\pi^2 \rho_g d_p^5 \left(\frac{\rho_p}{\rho_g}\right)^2 C_c} \tag{4}$$

 

where $T$ is the temperature of the fluid, $\nu$ is the kinematic viscosity, $k_B$ is the Boltzmann constant and $\rho_g$ is the gas density.

Therefore, the Brownian force amplitude can be restated as [9]:

$$F_{Brownian} = \frac{\zeta}{m_d}\sqrt{\frac{1}{\tilde{D}}\frac{2k_B T^2}{\Delta t}} \tag{5}$$

where $m_d$ is the mass of the particle and $\tilde{D}$ is the diffusion coefficient given as [8]:

$$\tilde{D} = \frac{k_B T C_c}{3\pi\mu d_p} \tag{6}$$

**3. Geometry and mesh structure**

The geometry of a straight pipe is created in Gambit software and used in this paper. The diameter of the pipe is considered 0.45cm in this paper [16]. The resolution of the mesh is an important issue for simulating the particle deposition. Figure 1 displays the created mesh at the inlet of the tube. Gambit software is used for generating the geometry and mesh in this paper.

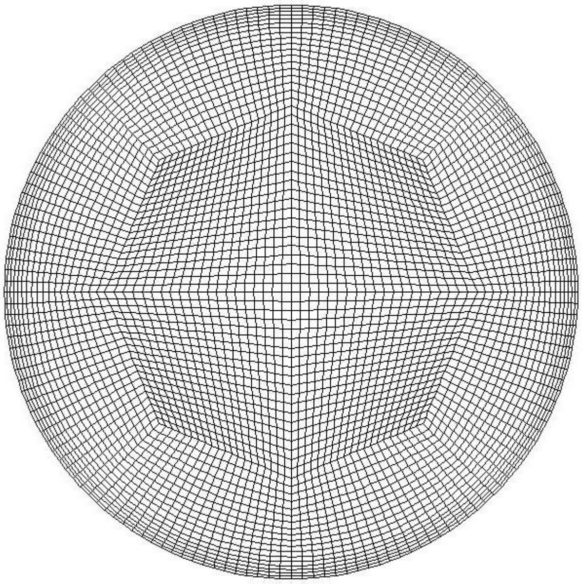

Figure 1. Mesh structure on the pipe inlet

As shown in this figure, dense mesh near the wall is necessary to determine the deposition efficiency correctly [17]. Note that the total number of nodes is about 800,000.

**4. Boundary conditions**

As mentioned before, the deposition efficiency is calculated in a fully developed flow in this paper. In order to achieve a fully developed flow in the straight pipe, an additional separate pipe with the length of 5D with the same cross section and mesh was simulated with periodic boundary condition. When the flow reached a fully developed state, the velocity profile of the outlet of the separate periodic straight pipe model was used as the inflow condition at the inlet of the main straight pipe [10]. The considered flow rates are 1 and 2 lit/min.

Boundary conditions for the particles were set up as a circular particle release entrained in the flow field. Particles were released from 0.01m from the inlet to prevent any spurious data exiting the inlet upon immediate release. In addition, the radial distance at which a particle was located was not less than 0.1 mm away from wall to eliminate artificial immediate deposition on the walls [10]. Note that 70,000 particles are injected randomly in order to reduce the statistical error of the predicted deposition efficiency. Note that higher number of particles are tested and almost no change is shown in the results. Furthermore, the 10 integration steps for Brownian motion are considered as the time step size [10].

## 5. Results and discussion

To verify the fluid flow simulation, the results of the flow simulations are compared with the exact solution for laminar pipe flow regime. The exact solution for the laminar flow in the cylinder is a parabolic profile for the velocity, which is given as [16]:

$$u(r) = 2u_{in}(1-\frac{r^2}{R^2}) \tag{7}$$

where $R$ is the pipe radius and $u_{in}$ is the mean velocity. Figure 2 compares the numerical velocity profile with the exact solution. It is seen that the two velocity profiles are identical.

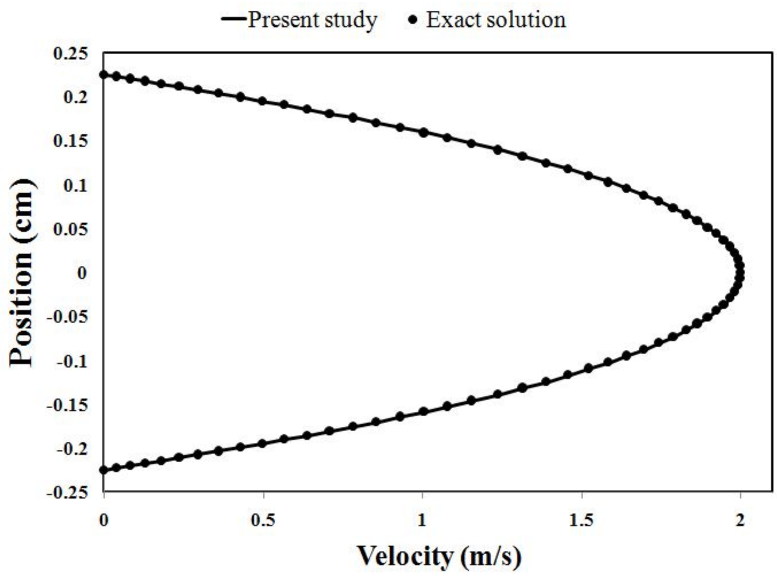


Figure 2. Comparison of the simulated velocity profile at the outlet with the exact solution

Figure 3 displays the velocity contour at the midsection of the cylinder. A fully developed flow pattern can be seen in this figure.

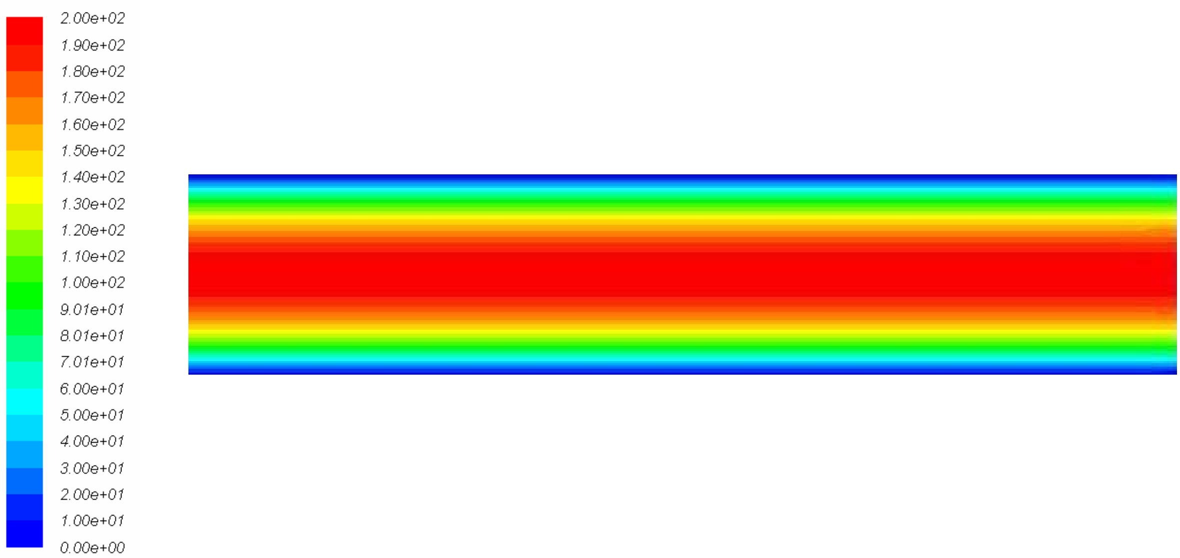

Figure 3. The velocity contour at the midsection of the pipe

Deposition results for the Brownian motion models are verified by comparing the results with different analytical expressions for the fully developed flow in pipes based on the diffusion parameter. Note that the point source analysis in a uniform flow is performed for validating the Brownian motion. The first employed equation was developed by Thomas [2] at 1976 which is calculated by the following equation:

$$DE = 1-(0.819e^{-14.63\Delta} + 0.097e^{-89.2\Delta} + 0.032e^{-228\Delta} + 0.027e^{-492\Delta} + 0.025e^{-3000\Delta}) \tag{8}$$

where $\Delta$ is the dimensionless diffusion parameter defined as [3]:

$$\Delta = \frac{\tilde{D}L_{pipe}}{4U_{in}R^2} \tag{9}$$

where Lpipe is the pipe length and R is the pipe radius.
The second employed equation is developed by Ingham at 1975 which is defined as follow [3]:

$$DE = 1-(0.819e^{-14.63\Delta} + 0.0976e^{-89.22\Delta} + 0.0325e^{-228\Delta} + 0.0509e^{-125.9\Delta^{2/3}}) \tag{10}$$

The third one is developed by Yeh and Schum [5] at 1980 which determined the deposition efficiency for laminar parabolic flow condition as following:

$$DE = 1-(0.819e^{-14.63\Delta} + 0.0976e^{-89.22\Delta} + 0.0325e^{-228\Delta} + 0.0509e^{-158.6\Delta^{2/3}}) \tag{11}$$

Note that the difference between the equation of Yeh and Schum with the Ingham equation is related to the last term in the equations.
Figure 4 displays the deposition efficiency calculated in the present paper in compare with the mentioned analytic equations for a pipe with the length of 1cm and a mean velocity of 1 m/s.

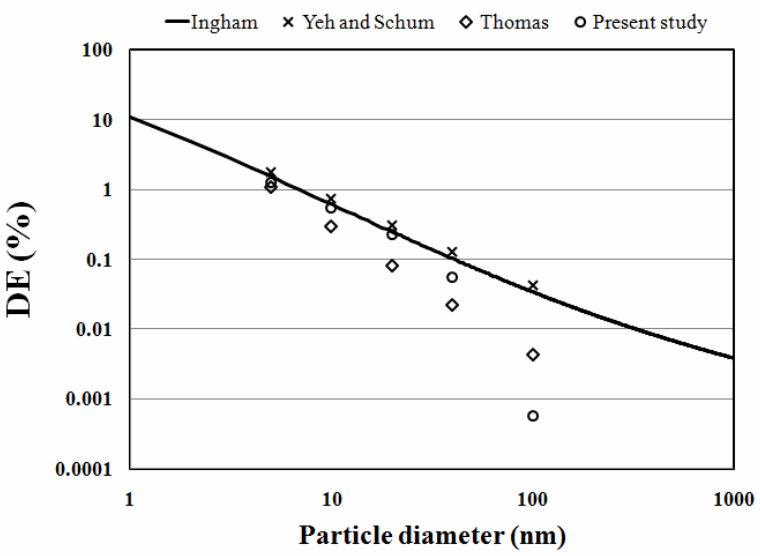


Figure 4. Comparison of the deposition efficiency for the 1cm long pipe and a mean velocity of 1m/s between the present result and the analytical expressions

It is seen that the presented results are in good agreement with the analytic equations.

The reason for the little difference may be due to the fact that the Lagrangian model is inherently transient, whereas the Eulerian model is a steady state approximation [7]. Furthermore, it should be noted that the results of different analytic correlations in litreture have also a little difference with each other. For larger particles, the difference may be explained by the increasing inertia of larger particles since the inertia effect cannot be considered in the Eulerian method or mass diffusion equation and this is another advantage of the direct Lagrangian method [7, 11].
Figures 5 and 6 display the deposition efficiency for cylinders with a lengths of 2 and 3 cm, respectively with the mean velocity of 1 m/s. As shown, for 100nm particles, due to the mentioned reasons, the calculated deposition efficiency is less than the value calculated from the analytic equations.

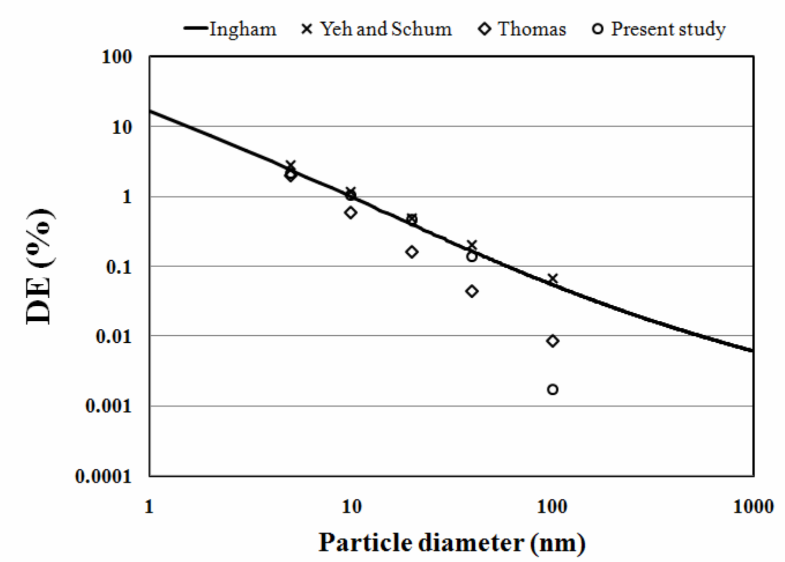


Figure 5. Comparison of the deposition efficiency for the 2cm long pipe with a mean velocity of 1m/s between the present result and the analytical expressions

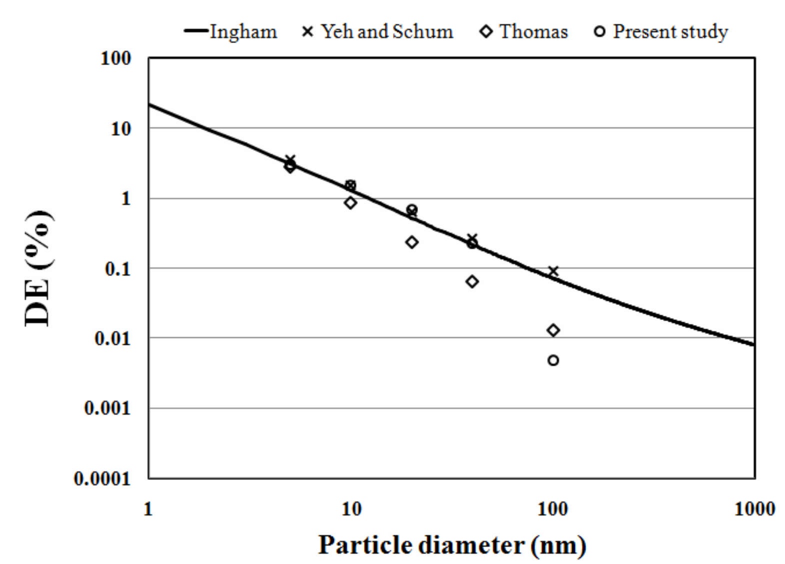


Figure 6. Comparison of the deposition efficiency for the 1cm long pipe with a mean velocity of 3m/s between the present result and the analytical expressions

For better understanding the effect of pipe length, Figure 7 shows the predicted deposition efficiency for different particle diameter and for different tube lengths of 1, 2 and 3cm with a mean velocity of 1 m/s. As displayed in the figure, the deposition efficiency is higher for the lower particle diameters due the higher Brownian force which effect motion of particles. Furthermore, by increasing the length of the pipe, the deposition efficiency is increased obviously.

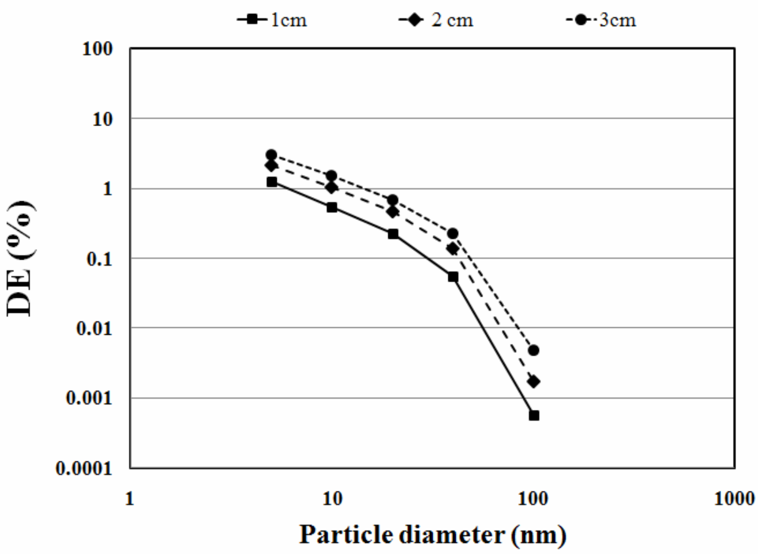


Figure 7. The deposition efficiency for cylinders with different lengths of 1, 2 and 3 cm and a mean velocity of 1 m/s

Figures 8-10 display the deposition efficiency for a pipe with the length of 5cm and different mean velocity of 0.5, 1 and 2 m/s in compare with the analytic equations. As displayed in Figure 8, decreasing the velocity causes a decrease in the inertia effect and therefore the deposition efficiency for the 100 nm particles is close to the analytic expressions. This is also can be seen in Figure 10 that by increasing the velocity and so on the inertia effect, the difference between the calculated deposition efficiency in this paper and the other analytical expressions increases.
For better understanding the effect of velocity, Figure 11 shows the predicted deposition efficiency for a pipe with the length of 5cm and different mean velocities of 0.5, 1 and 2 m/s calculated in this paper. As displayed, increasing the velocity cause that the particles leave the pipe faster and then the deposition efficiency decreases.

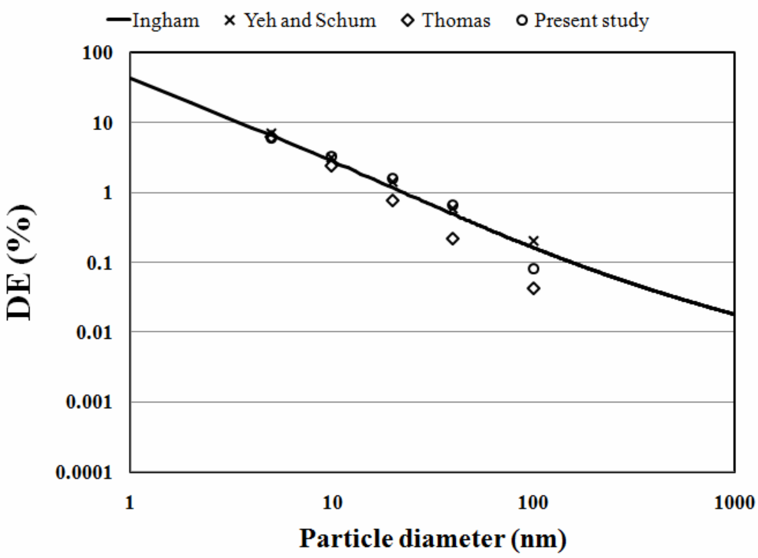


Figure 8. The deposition efficiency for a pipe with the length of 5 cm and a mean velocity of 0.5 m/s

 

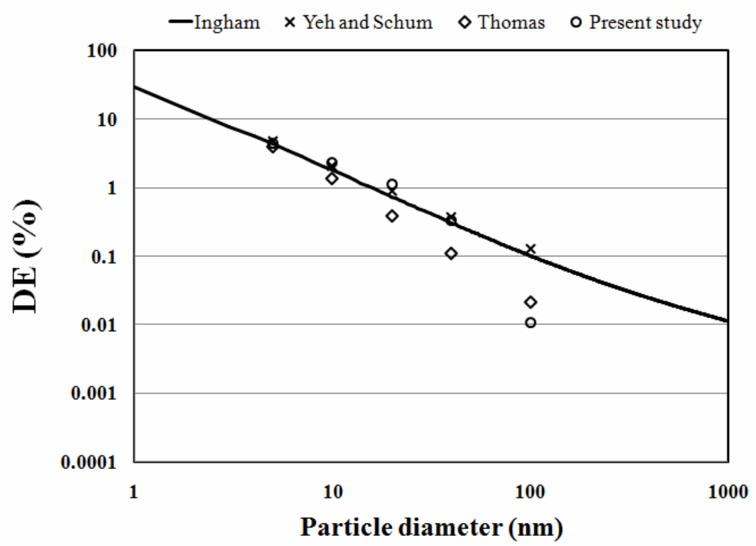


Figure 9. The deposition efficiency for a pipe with the length of 5cm and a mean velocity of 1 m/s

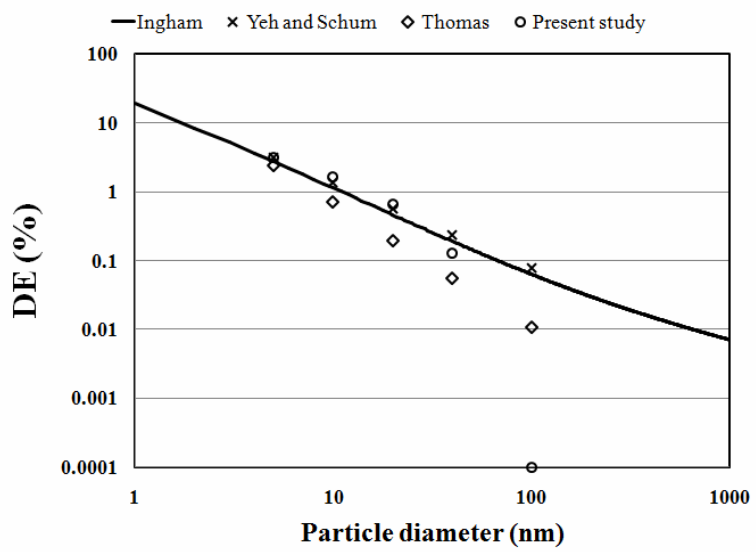


Figure 10. The deposition efficiency for a pipe with the length of 5cm and a mean velocity of 2 m/s

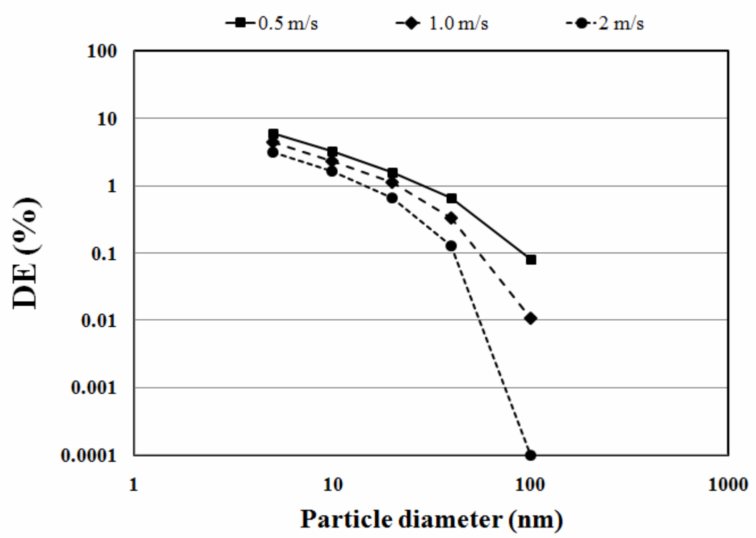


Figure 11. The deposition efficiency for a pipe with the length 5cm and different mean velocities of 0.5, 1 and 2 m/s

## 6. Conclusion

In this paper, the Lagrangian particle tracking method was employed to determine the deposition efficiency of nano-particles in cylindrical tubes. Different particle diameters, various flow rates and different pipe lengths were examined. The simulation results showed good agreement with the analytical expressions in the literature. It was also found that as the particles diameter or mean velocity increases, the deposition efficiency decreases in the pipe. Furthermore, for higher particle diameters, due to the effect of inertia or statistical error, the calculated deposition efficiency evaluated by the Lagrangian method deviates from the analytical correlations based on the diffusion.

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