CFD Study of Aerosol Particle Deposition in Converging-Diverging Nozzle

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Abstract

The particle deposition of turbulent flows in a 3D converging-diverging nozzle is numerically studied in this work. When particles are injected into the nozzle, the fluid-particle interaction is determined by the section diameter, flow conditions, particle diameter, and other factors. In this study, particle deposition in nozzles is simulated using the RNG *k-ε* turbulence model and the Lagrangian particle tracking model. At first, the mathematical model is verified by comparing with the experimental data of available literature. The particle diameter is varied from 2 to 9.5 micrometers in the simulation, with Stokes numbers ranging from 0.049 to 1.03 and Reynolds numbers ranging from 400 to 10,000. The present investigation shows how particle deposition efficiency is influenced by Stokes and Reynolds numbers in a converging-diverging nozzle and it is found that the nozzle's deposition efficiency increases slightly as the Stokes number increases.

Keywords
Deposition Efficiency, Converging-diverging nozzle, Stokes Number, Turbulent Flow, RNG *k-ε* turbulence model.

1. Introduction

Particle deposition is the continual attachment of particles to a surface as a result of favorable particle-surface interaction and hydrodynamic flow conditions. Due to its wide range of applications in biomedical, industrial, aerosol science, and other fields, particle deposition in a pipe has piqued the interest of many researchers. Because it stops the flow of air and affects the effectiveness of the operation, air particle deposition in a duct or pipe has gotten a lot of attention in the aerosol industry.

1.1 Literature Review

Many scholars have conducted experimental and numerical studies of particle deposition in various geometries and cross-sections for various particle sizes and Reynolds numbers. Pui *et al.* (1987) conducted an experimental research of air particle deposition in a circular 90° bend pipe with varying bend radius. They presented a correlation for particle deposition coefficient with the variation of Stokes number. Experiments were performed using monodispersed aerosols generated by the vibrating orifice aerosol generator at Reynolds numbers of 100 to 10,000 with bends constructed of stainless steel and glass tubes of different diameters.

After that, many researchers tried to simulate particle deposition in a circular 90° bend. A unifying correlation $\eta = (2/\pi)\tan^{-1} aSt^b$, where η is deposition efficiency and St is Stokes number for micron particle deposition in 90° bends with laminar flow was proposed by Inthavong (2019), but he did not account for the sedimentation effect. He varied Reynolds numbers from 400-2000 and particle diameters from 1-100 µm. He found that deposition for small particles was lower than that for large particles.

A similar kind of study was done by Guo *et al.* (2020) for square 90° bend pipe by varying Stokes number and keeping Reynolds number fixed at 10,000 via numerical simulation. According to Kim *et al.* (2014), they used RNG *k-ε* turbulence model for pipe flow simulation and the discrete phase model for particle simulation since the RNG *k-ε* turbulence model has a substantially lower computational cost and time than the RSM turbulence model. They showed a comparison of deposition between the circular and the square cross-sections of 90° bend pipe and discussed how the bend radius affected the particle deposition.

Sun *et al.* (2011) conducted a simulation for turbulent particle deposition in circular 90° bend pipe for Reynolds number of 17,900-35,600 and particle diameter of 1-4 μm. Particle deposition in circular 90° bend pipe was also investigated for various Reynolds numbers by Seyfi *et al.* (2020), Breuer *et al.* (2006), and Arsalanloo and Abbasalizadeh (2017). Apart from considering bend pipe/duct, Talebizadehsardari *et al.* (2020) simulated particle deposition in an annular pipe for flow of nanoparticles at Reynolds number of 10,000.

1.2 Objectives

From the above literature review, we can see that only circular 90° bends got higher priority from many researchers. However, no detailed study has been done considering particle deposition inside nozzles of different types. It is well known that the contraction and the expansion of pipe cross-sections are used for various purposes. Hence, particle deposition in the pipe with contraction and expansion section is the focus of this study, and it is our concern to investigate aerosol particle deposition in the converging-diverging nozzle.

2. Model and Governing Parameters

The present physical models consist of a converging-diverging nozzle with a straight-circular pipe attached to its entrance. The geometries of the models along with dimensions are shown in Fig. 1. The converging-diverging section is symmetrical in shape and a fillet of 10 mm is used at the junction of converging and diverging section. The diameter of straight section, D = 8.51 mm. Flow condition is assumed to be steady state throughout the study. Air is the working fluid and addressed as continuous and incompressible. The Euler-Lagrange multiphase flow model is used. Airflow is governed by the Eulerian conservation equations.
Injected particles are spherical, smooth, and diluted in terms of total volume. They are moving in a Lagrangian reference frame, and their movements do not have any impact on the air flow. That is why, one-way coupling is used to track the path of the particles.
Newton's second law helps to describe the movements of the particles as follows:

$$\frac{du_p}{dt} = F_d + \frac{g\left(\rho_p - \rho_g\right)}{\rho_p}, \tag{1}$$

where, u is the velocity, ρ is the mass density, g is the gravitational acceleration, the subscripts 'p' and 'g' indicate the particle phase and the gas (air) phase respectively. The equation is solved using Runge-Kutta discretization. F_d is the drag force per unit mass which can be determined using Stoke's resistance model,

$$F_d = \frac{18\mu}{\rho_p d_p^2}\frac{C_d\,\mathrm{Re}_r}{24}\left(u_g - u_p\right) = \frac{\left(u_g - u_p\right)}{\tau}, \tag{2}$$

where d_p is the particle diameter, μ is the dynamic viscosity of the fluid, τ is the relaxation time of the particle, Re_r is the relative Reynolds number, and C_d is the drag coefficient of the particle. Morsi and Alexander (2006) gave the definition of drag coefficient (C_d) as:

$$C_d = a_1 + \frac{a_2}{\mathrm{Re}_r} + \frac{a_3}{\mathrm{Re}_r{}^2}, \tag{3}$$

where a_1, a_2, a_3 are constants used for particles over different arrays of relative Reynolds number (Re_r). It can be defined as:

$$\mathrm{Re}_r = \frac{\rho_g d_p \left|u_p - u_g\right|}{\mu}, \tag{4}$$

In the same way, Reynolds number governing the flow can be defined as:

$$\mathrm{Re} = \frac{\rho_g u_m D}{\mu}, \tag{5}$$

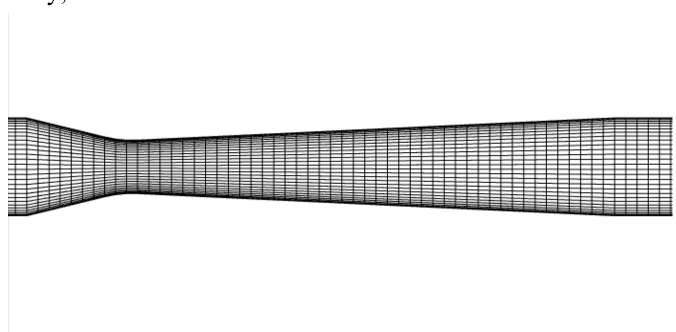
Equation (1) also contains some additional forces – Brownian force, Staffman's lift force, thermophoresis force, pressure gradient force, and virtual mass force. Brownian force and lift force become dominant for particles that have Nano level sizes. Particles injected in this study have a size range of 2-9.5 µm. So, we can neglect these two forces. Density of air is negligible to that of the particles. Throughout the study, no temperature related term is introduced. Because of these, we can safely neglect rest of the forces described above.
With time, a sticky scale may form inside the pipes. Particles become stuck as soon as they contact the wall. An experimental study conducted by Pui *et al.* (1987) suggests that in such scenarios, particle rebound should be ignored. As a result, 'trap' is chosen as the DPM boundary condition of the wall, whereas 'velocity inlet' and 'pressure outlet' conditions are used for inlet and outlet, respectively. The fluctuating velocity component influences particle trajectory during turbulent flow. To take this into account, discretized Random Walk Model is used, and Stochastic Particle Tracking governs the model.
The particles are injected a set distance of 8D from the inlet. It guarantees that no particles are left behind and that they are distributed evenly throughout the flow. Based on the Stokes number defined by Pui *et al.* (1987), multiple injections are introduced in the model.

$$St = \frac{C_c \rho_p d_p^2 u_m}{18\mu\left(D/2\right)}, \tag{6}$$

where u_m is the mean flow velocity, D is the hydraulic diameter and C_c represents the Cunningham correction factor defined as,

$$C_c = 1 + \frac{\lambda}{d_p}\left(2.514 + 0.8e^{-0.55 d_p/\lambda}\right), \tag{7}$$

where λ indicates the mean free path of air molecules.
Spherical particles of uniform diameters are injected in each injection. The velocity of release is similar to the speed of the continuous phase, i.e., the air. Based on Stokes number, particle size differs from one injection to another. In our study, the Stokes number varies from 0.049 to 1.03. The injected particles are inert, having a density of 895 kg/m^3. The dynamic viscosity and density of air are 1.7894×10^{-5} kg/ms and 1.225 kg/m^3, respectively. Turbulent intensity is limited to 5% in value. The wall has a no-slip boundary condition. Turbulence parameters have an effect on the region near the wall. As a result, the Enhanced Wall Treatment option is enabled to improve accuracy. A system's particle deposition rate can be evaluated using deposition efficiency, which is defined as follows:



$$\eta = \frac{N_{pt}}{N_{pe}}, \tag{8}$$

where N_{pt} is the number of particles trapped and N_{pe} is the number of particles entered in the system.

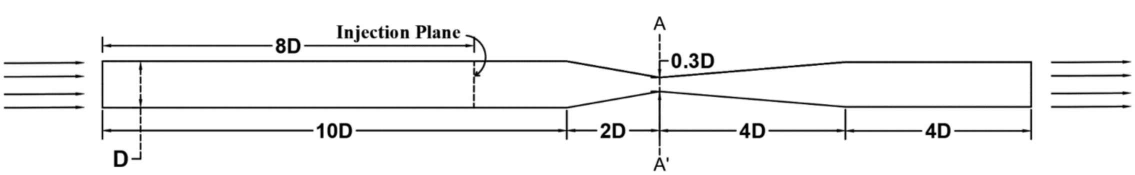
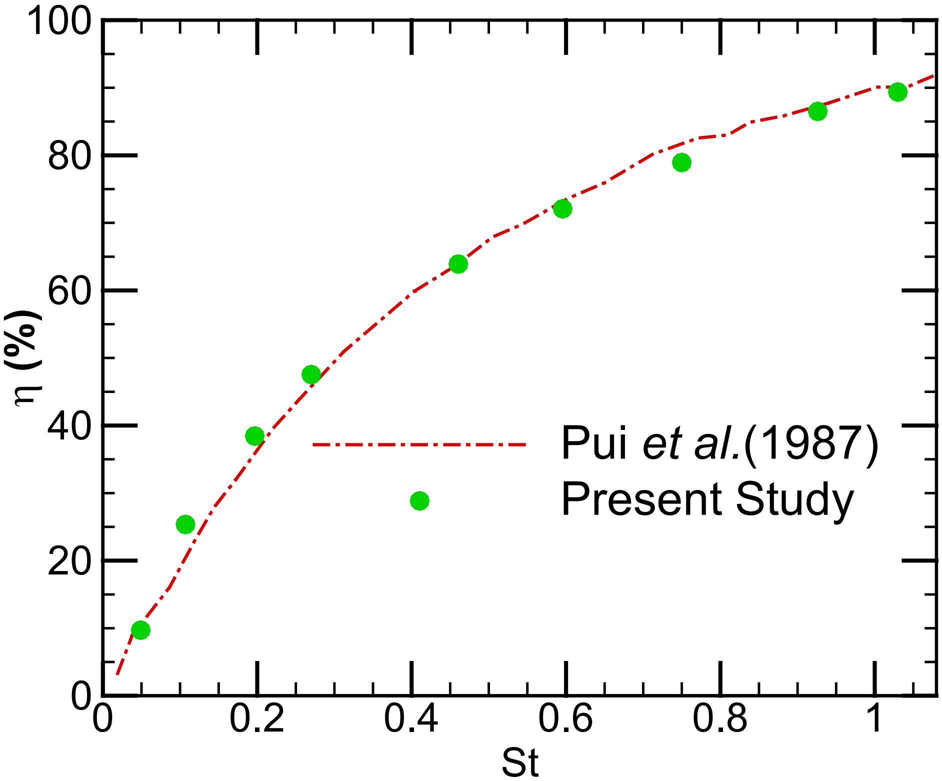


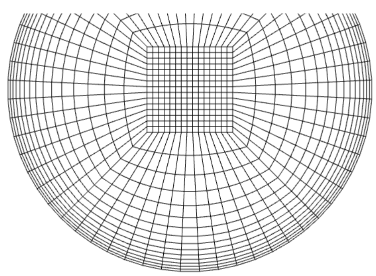
Fig. 1: Schematic diagrams of converging diverging nozzle with physical dimensions.

(a) (b)

Fig. 2: Meshed geometry of converging diverging nozzle (a) Cross section (b) Nozzle section.

3. Numerical Simulation and Validation





The finite volume method is used to discretize the computational domain, and ANSYS FLUENT is used to solve the corresponding governing equations. O-type structured mesh of the model is shown in Fig. 2. It helps to get an easy-to-control mesh near the wall and improves the accuracy of the results. The laminar flow model is considered for a Reynolds number of 400. On the other hand, the RNG k-ε turbulence model is considered for Reynolds number 4000 and higher. There are several turbulence models available. But Kim *et al.* (2014) found that results obtained by using the RNG k-ε model provide sufficient accuracy. Pressure-velocity coupling is implemented using the COUPLED algorithm. The algorithm is a pressure-based one. The second-order upwind scheme is used to discretize the momentum, pressure, turbulent kinetic energy, and dissipation rate. A residual of 10^{-5} is selected as the criterion for convergence for all the variables.

In agreement with their physical model and flow conditions (90º bend circular pipe with a diameter of 8.51 mm, curvature ratio = 5.6, Re = 10,000, ρ_p = 895 kg/m^3 and d_p = 2-10 μm), the current model is validated against the experimental study conducted by Pui *et al*. (1987). Their study suggests that deposition efficiency and Stokes number can be related using the following equation:

$$\eta = \left(1 - 10^{-0.963\,St}\right) \times 100\%, \tag{9}$$

As illustrated in Fig. 3, the numerical simulation produces results that are similar to those obtained in the experimental work. As a result, it can be confidently inferred that the existing simulation method is legitimate and reliable.

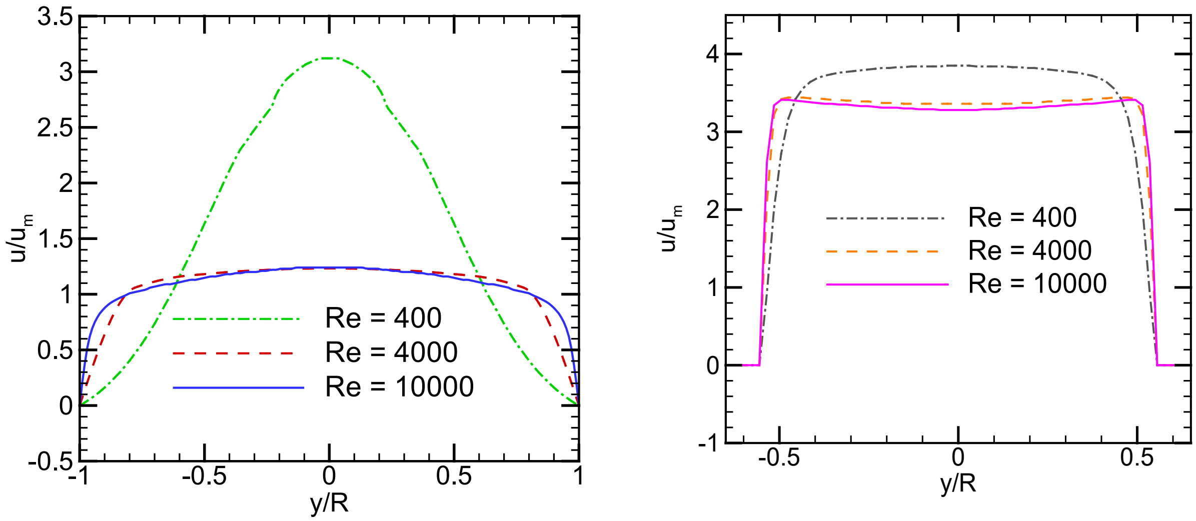


Fig. 3: Validation of the present model in terms of particle deposition efficiency as a function of Stokes number with the experimental investigation in 90° circular bend by Pui *et al.* (1987).

4. Results and Discussion

The velocity profiles at the outlet and A-A' for Re = 400, 4000, and 10,000 are plotted in Fig. 4 for the converging-diverging nozzle. Velocity profiles for laminar and turbulent flows have an almost similar flat shape at the junction of the converging and diverging sections, and the flow velocity at that section is higher than the mean velocity for each Re that is considered. But, at the outlet, fully developed laminar flow is indicated by the parabolic shape, and the velocity at the pipe center is higher than the mean velocity. Whereas flat velocity profiles are seen for turbulent flows, this time the velocity is close to the mean velocity.

(a) (b)

Fig. 4: Velocity profiles at (a) outlet and (b) A-A' Section of the converging-diverging nozzle for *Re* = 400, 4000 and 10,000.

(c) (d)

Fig. 5: Turbulent kinetic energy profiles at (c) outlet and (d) A-A' section of the converging-diverging nozzle for *Re* = 4000 and 10,000.

Fig. 5 shows the fluctuation of turbulent kinetic energy for more turbulent flow at the A-A' section, whereas stable profiles for turbulent kinetic energy can be found at the outlet.

A quantitative assessment of particle deposition is carried out by showing deposition efficiency as a function of Stokes number for a converging diverging nozzle and a straight pipe with a similar diameter at *Re* = 10,000 (Fig. 6). As can be seen from equation (6), the Stokes number varies with particle diameter in this case because the mean flow velocity is fixed for *Re* = 10,000. With particle sizes ranging from 2 to 9.5 µm, the Stokes number varies from 0.049 to 1.03. For a given Stokes number, deposition efficiency is always higher in a pipe with a converging-diverging nozzle than in a straight pipe. In the straight circular pipe, the deposition efficiency is significantly lower and gradually increases as the particle diameter increases. The deposition efficiency increases slightly and remains around 45% for the Stokes number range in a converging-diverging nozzle. For the straight circular pipe, the highest deposition efficiency is around 23% for particles with a diameter of 9.5 µm, which is nearly half that of the converging-diverging nozzle.

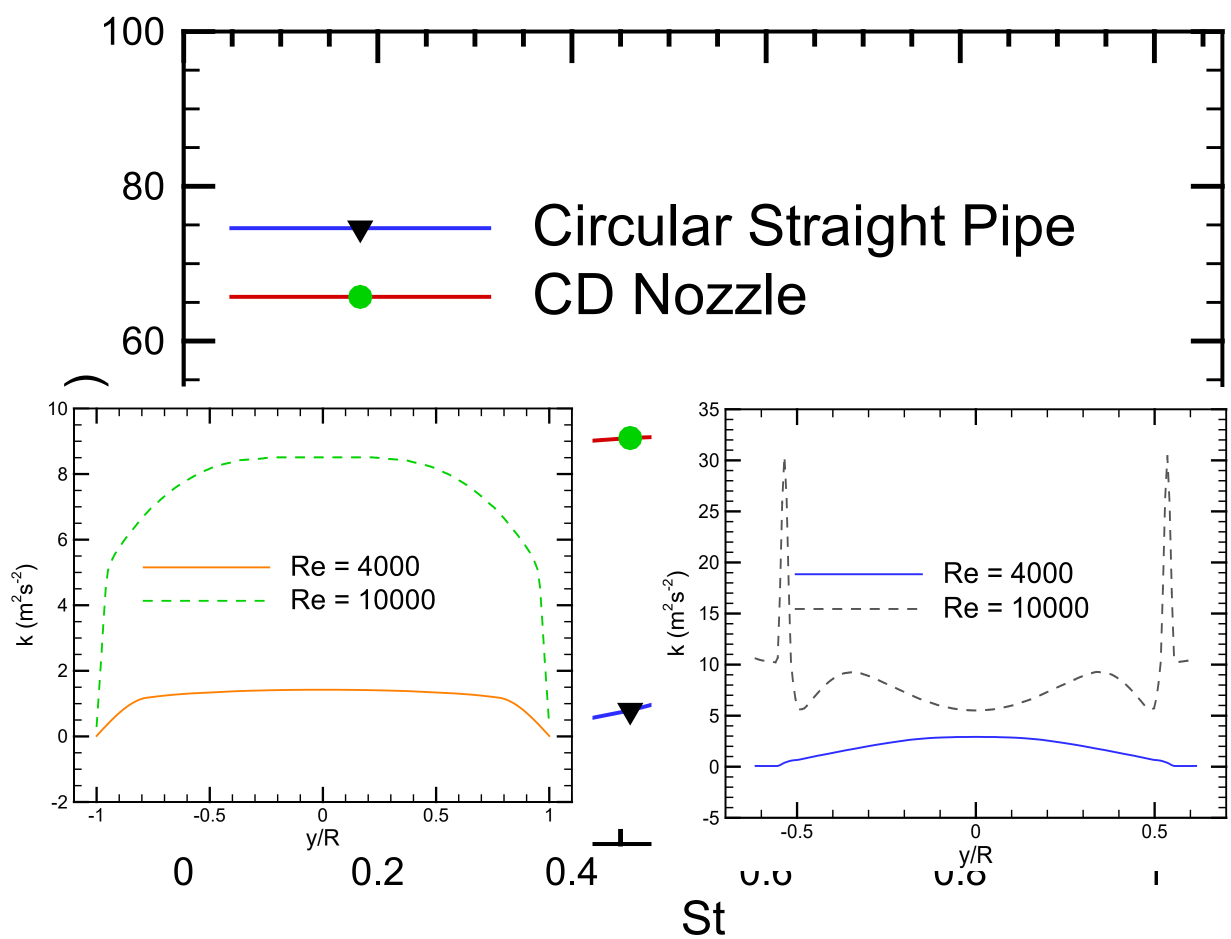
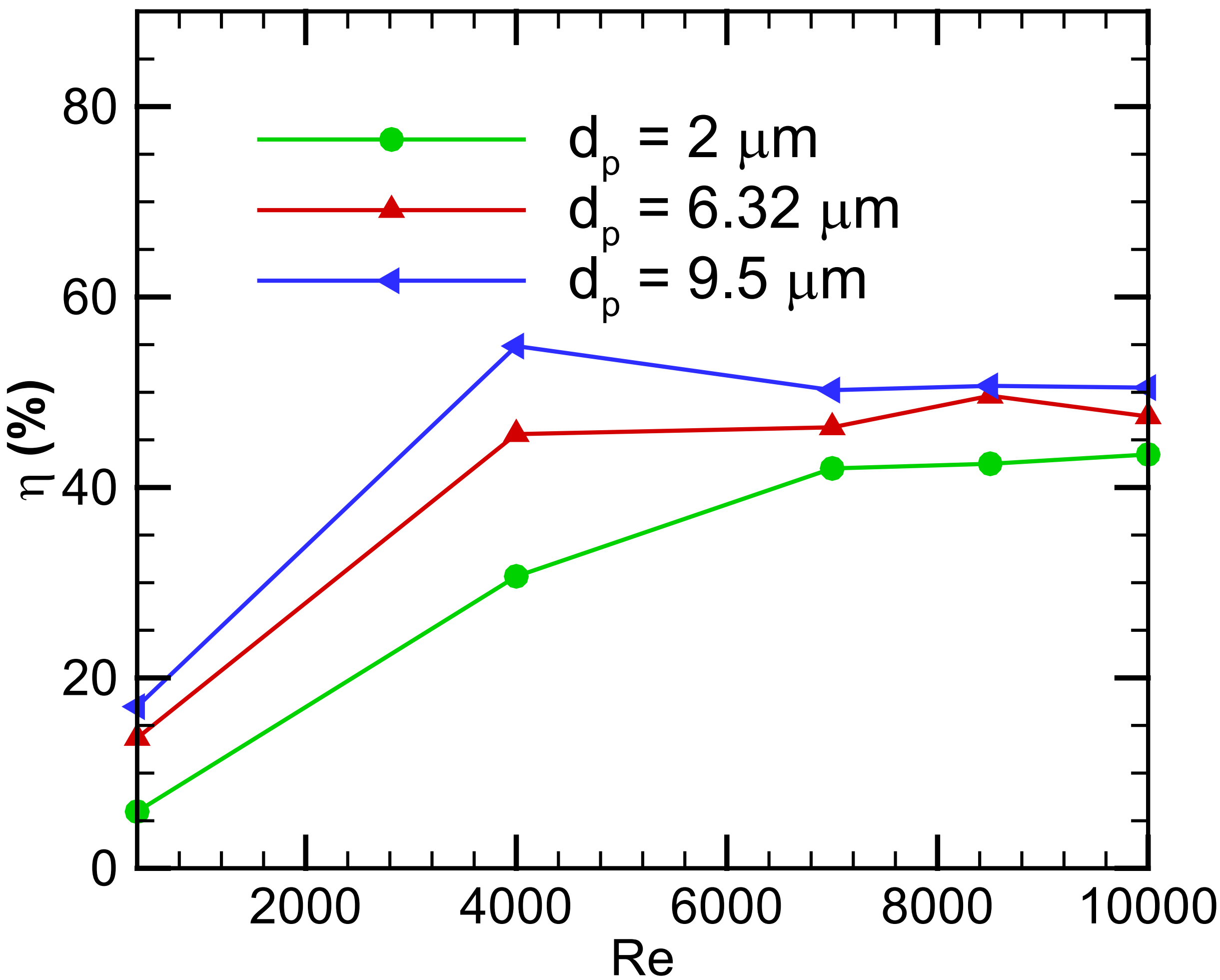


Fig. 6: Variation of deposition efficiency with particle Stokes Number for converging diverging nozzle and straight pipe at *Re* = 10,000.

Another variation of deposition efficiency as a function of *Re* is plotted in Fig. 7 for particle diameters of 2, 6.32, and 9.5 µm. For turbulent flows, deposition efficiency increases with increasing *Re* and remains almost stable afterwards. For a given *Re*, deposition efficiency is higher for particles with a larger diameter, whereas for laminar flow, deposition efficiency is considerably lower for each of the three particle diameters considered.

Fig. 7: Variation of deposition efficiency with Reynolds number for at d_p = 2, 6.32, 9.5 µm for the converging-diverging Nozzle.



5. Conclusion

The ANSYS FLUENT program is used to model particle deposition in a converging diverging nozzle. Eulerian-Lagrangian multiphase flow model is used for its higher efficiency. To estimate the air and particle flow, the RNG k-ε turbulence model and the Lagrangian stochastic tracking model have been used, correspondingly. Before executing the numerical simulation of the current problem, the numerical approach is validated against a previously published experimental work. The following conclusion can be made based on this comparative study:

- Particle deposition efficiency is not largely varying with particle diameter, rather increases slightly in converging diverging nozzle and stays around 45% for *Re* = 10,000.
- For straight circular pipe, deposition efficiency increases with particle diameter for a particular flow.
- For a given *Re*, larger diameter particles have a higher deposition efficiency.
- Higher particle deposition efficiency is observed for converging-diverging nozzle than straight pipe.

- Deposition efficiency is substantially lower in laminar flow and does not change much. However, it increases with increasing *Re* for turbulent flows.

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References
Arsalanloo A and Abbasalizadeh M. 2017. Numerical study on deposition of particles in a 90° bend in the presence of swirling flow using eulerian-lagrangian method. *Powder Technol.,*320: 285-294.

Breuer M, Baytekin HT and Matida EA. 2006. Prediction of aerosol deposition in bends using les and an efficient lagrangian tracking method. *Aerosol Sci. Technol.,*37(11): 1407-1428.

Guo J, Chen Z, Shen B, Wang J and Yang L. 2020. Numerical study on characteristics of particle deposition efficiency on different walls of 90° square bend. *Powder Technol.,* 364: 572-583.

Inthavong K. 2019. A unifying correlation for laminar particle deposition in 90-degree pipe bends. *Adv. Powder Technol.*,345: 99-110.

Kim J, Yadav M and Kim S. 2014. Characteristics of secondary flow induced by 90-degree elbow in turbulent pipe flow. *Poromechanics V* (*2013*)*,* 8(2): 229-239.

Morsi SA and Alexander AJ. 2006. An investigation of particle trajectories in two-phase flow systems. *J. Math Fluid Mech.,* 55(02).

Pui DYH, Romay-Novas F and Liu BYH. 1987. Experimental study of particle deposition in bends of circular cross section. *Aerosol Sci. Technol.,*7(3): 301-315.

Seyfi S, Mirzayi B and Seyyedbagheri H. 2020. Cfd modeling of black powder particles deposition in 3d 90-degree bend of natural gas pipelines. *J. Nat. Gas Sci. Eng.,*78.

Sun K, Lu L and Jiang H. 2011. A computational investigation of particle distribution and deposition in a 90° bend incorporating a particle–wall model. *Build Environ.,* 46(6): 1251-1262.

Talebizadehsardari P, Rahimzadeh H, Ahmadi G, Inthavong K, Keshtkar MM and Moghimi MA. 2020. Nano-particle deposition in laminar annular pipe flows. *Adv. Powder Technol.*,31(8): 3134-3143.

Biographies

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