Numerical simulation of aerosol deposition from turbulent flows using three-dimensional RANS and LES turbulence models

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In this study, three-dimensional computational fluid dynamics (CFD) simulations of particle deposition from turbulent flows in a vertical straight pipe were carried out, using the STAR-CCM + v5.04 CFD package. The highlight of the study is the development of a post-processing approach for quantitatively assessing the accuracy of the Lagrangian particle tracking scheme. Three Reynolds-averaged Navier–Stokes (RANS) models and a large eddy simulation (LES) model were employed in the simulations, in conjunction with two wall treatment schemes and several near-wall mesh conditions. The particle deposition velocity was obtained based on the CFD simulation results, and compared to the experimental results. In post-processing, a “particle responsiveness factor,” defined as the ratio of particle mean square velocity fluctuation to fluid mean square velocity fluctuation for the wall-adjacent cells, was quantified using an Eulerian particle transport formulation. The particle responsiveness factor of the CFD simulations was then compared with that obtained using an empirical equation. The most accurate aerosol deposition results were obtained with a fine near-wall mesh (y⁺ ≈ 1) and resolved near-wall flow (no wall function). The LES model and the Reynolds stress model (RSM) produced the most accurate deposition velocity results, but the computation time of the former was up to ten times longer than that of the latter. The lower accuracy of the isotropic RANS models was attributed to their overprediction of the near-wall turbulence intensity gradient, and less accurate particle tracking as suggested by the particle responsiveness factor. The particle responsiveness factor, introduced for the first time in this study, was shown to be a useful index for evaluating accuracy of the Lagrangian particle tracking scheme due to its independence of specific knowledge of CFD algorithm and coding.

Keywords: RANS; LES; turbulence; aerosol deposition

Introduction

For aerosol particles in a turbulent flow, the interaction between particles and fluid eddies leads to particle transport and deposition. In a wide range of industrial applications and environmental processes, turbulent transport is a major mechanism of particle deposition (Davies, 1966; Hinds, 1999). Experimental studies of turbulent deposition in pipe flows have resulted in some useful empirical relations (Friedlander & Johnstone, 1957; Liu & Agarwal, 1974; Papavergos & Hedley, 1984). There has also been a strong interest in using computational fluid dynamics (CFD) simulations to quantify aerosol deposition in turbulent flows. The early CFD models for turbulent aerosol deposition utilize the “two-fluid” Eulerian approach. In such models, particle transport in the bulk flow is by turbulent diffusion. At a characteristic distance from the wall, the particle concentration is assumed to vanish. The characteristic distance is typically assumed to be one-particle stop distance, which is a function of particle relaxation time and wallward velocity (Davies, 1966; Friedlander & Johnstone, 1957). With the advancement of computational power, the use of Lagrangian models, represented by the eddy interaction model (EIM) (Graham, 1996; Gosman & Ioannides, 1983), has become common in CFD simulation of particle transport and deposition in turbulent flows.

Over the years, various modifications to the EIM have been introduced to better simulate fluid physics, and hence improve accuracy of the Lagrangian particle tracking model. For example, shear-induced lift causes a particle to move faster and further in the wallward direction than it would in the absence of shear. Therefore, incorporating shear-induced lift force in the EIM may improve simulation accuracy, especially when the dimensionless relaxation time τ + is large and the particle/fluid density ratio is small (Kallio & Reeks, 1989). To improve the “standard” EIM, Graham (1996) introduces a modification that allows the maximum fluid-particle interaction time to exceed the eddy lifetime. This modification results in improved accuracy of the simulated particle dispersion coefficient.

EIM would not be useful without accurate description of the turbulent flow field. For example, the near-wall turbulent flow is anisotropic by nature, but Reynolds
Average Navier–Stokes (RANS) turbulence models depict turbulence as isotropic. As a result, EIM in conjunction with these models leads to unsatisfactory turbulent deposition simulation results (Matida & Nishino, 2000). “Correction” may be introduced, i.e., in the form of a damping method, for isotropic turbulence models to better simulate turbulence in the near-wall region, and hence obtain improved particle deposition simulation (Wang & James, 1999). CFD-grid resolution is of great importance for accurate particle tracking, especially in the near-wall region. This is particularly the case for small particles, as their deposition is governed by the flow properties of the near-wall layer. For large inertial particles turbulent dispersion in the bulk flow plays an important role in deposition (Uijttewaal & Oliemans, 1996). When using Large Eddy Simulation (LES) for simulation of particle transport in turbulent flow, the significance of sub-grid-scale (SGS) velocity fluctuation must be taken into consideration. Neglecting SGS velocity fluctuations would lead to error. At higher Reynolds number or lower grid resolution, the effect of SGS velocity fluctuation becomes more pronounced. Because small particles respond to a relatively broad spectrum of turbulent motions, the greatest error occurs for particles possessing the smallest relaxation times (Wang & Squires, 1996).

Not surprisingly, studies using various commercial CFD models have confirmed the general findings obtained using academic codes. For example, the turbulence model and the near-wall mesh resolution are the two most important parameters. A Reynolds stress model (RSM) with the proper wall treatment would lead to the most accurate simulation of particle deposition velocity, while a k-ε turbulence model would overpredict particle deposition velocity due to overprediction of wall-normal turbulent fluctuation. The mesh resolution needs to be sufficiently fine such that the y* value of the wall-adjacent cells is on the order of 1 (Parker & Foat, 2008; Tian & Ahmadi, 2007).

Overall, the shortcomings of RANS turbulence models and the limitations of the EIM particle tracking approach have been well documented in the literature, and various model modifications have been proposed to address the problems. The modifications are in general successful in what they are intended to address. However, there has been a lack of research in how to assess turbulent aerosol deposition models on a common basis. This is especially true for CFD models that involve proprietary codes. Without a common basis to evaluate these model modifications, it is difficult to identify directions for future improvement. For example, specific model modifications may lead to either under-prediction or over-prediction of the deposition velocity (Kallio & Reeks, 1989; Nicoud & Ducros, 1999; Parker & Foat, 2008; Tian & Ahmadi, 2007; Wang & James, 1999; Wang & Squires, 1996). Without a common basis for model performance evaluation, it would be impossible to know what modifications should be preserved and developed for general applications beyond pipe flows. In view of this, there is a need to develop methods that can be used to evaluate turbulent deposition models based on the fundamental physics.

The objective of this study is to develop such an evaluation method. In this study, we carried out 3-D simulations using a commercial CFD model that had not been reported for the simulation of turbulent deposition. In this process, we applied existing knowledge of the effects of CFD parameters in setting up the simulation. Our focus was to develop a quantitative method for assessing the accuracy of the CFD package’s particle tracking scheme. To that end, we quantified the CFD model’s particle tracking performance in terms of a “particle responsiveness factor” (defined in the Methods of Post-Processing section), and compared the CFD model’s particle responsiveness factor with that calculated using an empirical relation. In the ensuing sections, the relevant theory, the methods and the results are described, and the significance of the results is discussed.

**Theory**

Empirical relations of turbulent deposition are typically presented in terms of the dimensionless particle relaxation time τ+ and the dimensionless deposition velocity V+. The dimensionless particle relaxation time is based on the particle relaxation time (Hinds, 1999). For a spherical particle, the particle relaxation time is defined as:

\[
\tau = \frac{\rho_p d_p^2 C_c}{18 \mu}
\]

where \(\rho_p\) is the particle density, \(d_p\) is the particle diameter, \(C_c\) is the Cunningham slip correction factor, and \(\mu\) is the dynamic viscosity of the fluid. The dimensionless particle relaxation time is then defined as:

\[
\tau_+ = \frac{\tau u^*}{\nu}
\]

where \(u_*\) is the friction velocity (Landau & Lifshits, 1987) defined in Equation (3), and \(\nu\) is the kinematic viscosity. The friction velocity is given by:

\[
u_* = \left(\frac{f}{2}\right)^{0.5} U
\]

where \(U\) is the average fluid velocity and \(f\) is the Fanning friction factor for the pipe flow. For the smooth pipe used by Liu and Agarwal (1974), the friction factor is calculated from the Blasius formula given by Schlichting (1968), valid for \(Re < 100,000\):

\[
f = \frac{0.316}{4Re^{0.25}}
\]

where \(Re\) is the pipe flow Reynolds number based on the pipe inner diameter.
The dimensionless deposition velocity $V_+ = \frac{V_{\text{dep}}}{u_*}$ is the ratio of the deposition velocity $V_{\text{dep}}$ to the friction velocity (Lee & Gieske, 1994; Liu & Agarwal, 1974):

$V_+ = \frac{V_{\text{dep}}}{u_*}$ (5)

For turbulent deposition in pipe flows, the following regimes have been observed (Guha, 1997, 2008):

- **Regime I** ($\tau_* < 0.3$): Particles follow the flow almost perfectly; deposition is dominated by Brownian motion; deposition velocity $V_+$ decreases as $\tau_*$ increases, and may be described with a turbulent version of Fick’s law of diffusion.
- **Regime II** ($0.3 < \tau_* < 30$): Particle “slip” relative to the flow is significant, and particle motion is strongly dependent on turbulent fluctuation in the fluid flow; deposition velocity $V_+$ increases as the second power of $\tau_*$.
- **Regime III** ($\tau_* > 30$): Particles have large inertia and the effect of turbulence on particle motion is significantly reduced; deposition velocity $V_+$ decreases with increasing particle size.

Guha (1997, 2008) has proposed an Eulerian description of particle transport in turbulent flow. This analytical description includes turbophoresis, i.e., particle transport due to gradient in turbulent velocity fluctuation. It also includes other mechanisms of particle transport such as thermophoresis, shear-induced lift force, electrical forces, and gravitational effects. A Cartesian coordinate system is adopted in Guha’s formulation, with the $x$ axis in the direction of the flow and the $y$ axis perpendicular to the wall. The particle convective velocity perpendicular to the wall (i.e., the deposition velocity), $\bar{V}_c$, is given in the following particle momentum equation:

$$\bar{V}_c \frac{d}{dy} \left( \bar{V}_c \right) + \frac{\bar{V}_c}{\tau_I} = - \frac{d}{dy} \left( \bar{V}_y^2 \right) + F_y$$ (6)

where $\tau_I$ is the particle inertial relaxation time, defined as:

$$\tau_I = \frac{24}{\tau Re_s C_D} C_c$$ (7)

where $\tau$ is the particle relaxation time, and $C_D$ is the Cunningham correction factor; $C_D$ is the drag coefficient, given by the following empirical relation (Clift & Grace, 1978). For small particles and low “slip” velocity between the particle and the gas flow, $\tau$ and $\tau_I$ are essentially equal.

$$C_D = \frac{24}{Re_s} (1 + 0.15Re_s^{0.687})$$ (8)

where the slip Reynolds number is defined as $Re_s = \frac{|u_f - u_p|d_p}{v}$.

The term $F_y$ is the $y$-component of forces acting on the particles, such as electrical force. The term $\bar{V}_y^2$ is the mean square velocity fluctuation of the particles in the $y$ (wall-normal) direction, and the term $- \frac{d}{dy} (\bar{V}_y^2)$ represents the turbophoresis effect. In general, the particle mean square velocity fluctuation $\bar{V}_y^2$ is not the same as the mean square velocity fluctuation of the gas flow $\bar{V}_y^2$.

This theoretical description of turbulent deposition was used in post-processing of the simulation results in this study, as described in the following section.

**Methodology**

In this study, we carried out flow field simulation using a quarter geometric model of the pipe flow, and Lagrangian particle tracking with the one-way coupling assumption. The one-way coupling assumption is that the gas flow field determines the particle motion, but the presence of particles does not affect the gas flow field. In post-processing of the simulation results, we used the Eulerian description of turbulent deposition introduced above to calculate the particle responsiveness factor. Herein we describe the methods of CFD simulation of turbulent deposition, and the post-processing methods.

**Methods of CFD simulation**

In this study, CFD simulation of turbulent deposition was carried out using the commercial code STAR-CCM + 5.04 (CD-adapco, London, UK), with the effects of several CFD parameters investigated. The simulation results were compared to experimental results of Liu and Agarwal (1974) for assessment of accuracy.

1) **Control volume and mesh generation**

The vertical straight pipe used in Liu and Agarwal’s experiment had a length of 1.02 m and an inner diameter of 12.7 mm. Taking advantage of the axisymmetric nature of the flow, a quarter cylindrical control volume was used for the CFD simulation in this study, representing one-fourth of the pipe flow. A three-dimensional geometric model was built using the STAR-CCM + geometry function (3D-CAD models).

For mesh generation, polyhedral cells with a target size of 0.1 mm were used for the bulk of the control volume. Prism cell layers were applied in the near-wall region, with the layer thickness increasing away from the wall at a growth factor of 1.1. Either 10 or 15 layers of prism cells were used. The wall-adjacent layer thickness was varied to examine the effect of wall treatment. For the High-$y_*$ Wall Treatment and the All-$y_*$ Wall Treatment in STAR-CCM + were applied to examine the effect of wall treatment. Wall treatment is often used in CFD simulation to model near-wall velocity in turbulent
Table 1. CFD-simulated turbulence gradient and particle deposition velocity results with various near-wall mesh settings (RSM model, all $y_+$ wall treatment unless otherwise noted, $Re = 10,000$), where $K_+ = K/u_+^2$.

| Number of prism layers | First layer thickness ($\mu$m) | Wall $y_+$ (first layer cell) | $K_+/y_+$ | $V_+$ at $\tau_+ = 1$ |
|------------------------|-------------------------------|-------------------------------|-----------|-------------------|
| 15                     | 5 $\mu$m                      | 0.25                          | 0.357     | 0.0014            |
| 15                     | 5 $\mu$m (High-$y_+$)         | 1.25                          | 0.438     | 0.0064            |
| 5 $\mu$m               |                               |                               | 0.405     | 0.0029            |
| 25 $\mu$m              |                               |                               | 0.428     | 0.0059            |
| 50 $\mu$m              |                               |                               | 0.416     | 0.0038            |
| Liu and Agarwal (1974) |                               |                               |           | 0.00112           |

For the all-$y_+$ wall treatment, it is recommended to have $y_+$ value on the order of unity. At locations where $y_+ < 5$, no wall function is used and the selected turbulent model is applied down to the wall-adjacent cells (CD-adapco, 2008). For the pipe flow in Liu and Agarwal’s study, a wall distance of 5 $\mu$m would give a unity $y_+$ value at Reynolds number of 50,000, and a $y_+$ of 0.25 at Reynolds number 10,000. Therefore, in this study the distance from the wall to the center of the first layer of prism cells was varied from 5 $\mu$m to 50 $\mu$m (corresponding to a $y_+$ value of 0.25 to 2.5 at $Re = 10,000$, and a $y_+$ value of 1 to 10 at $Re = 50,000$) to explore the effect of near-wall mesh resolution on turbulent deposition prediction.

(3) Boundary conditions

For the surface representing the wall of the pipe, the boundary condition was set to be “wall” with no-slip condition. In accordance with the experimental installation used by Liu and Agarwal (smooth glass pipe), the pipe wall boundary condition was set to be smooth. The inlet surface of the control volume was assigned “velocity inlet” boundary condition with a uniform velocity (11.84 m/s at $Re = 10,000$ and 60 m/s at $Re = 50,000$) perpendicular to the inlet surface, and a turbulence intensity of 0.1. The magnitude of the velocity was calculated from the flow rate used by Liu and Agarwal. The outlet surface of the control volume assigned “flow-split outlet” boundary condition, with a flow-split ratio of 100%. The two lateral boundaries were set to be connected “periodic plane” condition, following the axisymmetric simplification mentioned earlier in building of the pipe geometry model. For the particle phase, an “escape” boundary condition was assigned, i.e., no reflection or bounce for particles was allowed at the surfaces of the control volume.

(4) Turbulence modeling

Four widely used turbulence models available with STAR-CCM + were used in this study, namely the realizable k-ε model, the k-ω shear stress transport (SST) model, the Reynolds Stress model (RSM), and the Large Eddy Simulation model (LES). In this study, a maximum 5000 iterations was allowed for each simulation (all momentum residuals became almost constant and less than $10^{-3}$). When running the LES model, the flow field solution...
obtained with the RSM model was used as the initial solution. A time step of either 1 μs or 5 μs was used, and total of 5,000 ~ 10,000 time steps were completed to get the particle deposition results. The stopping criterion was either the simulation had reached 50 internal iterations within one time step, or the calculated residuals had all become lower than $10^{-4}$ of the initial residuals.

Two sub-grid-scale (SGS) models are available within STAR-CCM+: the Smagorinsky-Lilly model (1963) and the wall-adapting locally eddy-viscosity (WALE) model (Nicoud & Ducros, 1999). In the present work, the WALE model was employed for the final deposition results because of its advantages over the Smagorinsky model. The WALE model is based on the square of the velocity gradient tensor ($\mathbf{g}_{ij} = \frac{\partial u_i}{\partial x_j}$) and accounts for the effect of both the strain and the rotation rate to obtain the local eddy viscosity (Nicoud & Ducros, 1999). The WALE model, unlike the Smagorinsky model, needs neither a damping function nor a dynamic procedure to account for the no-slip condition at the walls (Jayaratne, Brouns, & Lacor, 2008). Also, the WALE model is apparently less sensitive to the value of the model coefficients than the Smagorinsky model (CD-adapco, 2008).

(5) Particle tracking

Particle trajectories were simulated following the turbulent flow field simulation, and it was assumed that the aerosol was sufficiently dilute and thus particles had no influence on each other or on the air flow (Tang & Guo, 2010). The Lagrangian multiphase model (also known as Lagrangian particle tracking) in STAR-CCM+ was applied to simulate the particle trajectories, in which the momentum equation of individual particles was numerically solved (Tang & Guo, 2011). Electrostatic forces, shear-induced lift forces, Brownian motion and thermophoresis were not included in this simulation. Particle diameter was varied from 1 to 20 μm in this study, corresponding to dimensionless relaxation time from 0.1 to 43 at Reynolds number 10,000, and dimensionless relaxation time from 2 to 740 at Reynolds number 50,000. The particle density was set to be 920 kg/m³ (olive oil), as was the case in Liu and Agarwal’s experiments (1974). Particles were released from a “surface injector” on the inlet boundary of the pipe at an initial velocity equal to the mean flow velocity; there were approximately 1000 uniformly distributed injection points on the surface injector.

Within the Lagrangian tracking approach, the CFD code predicted the turbulent dispersion of particles by integrating the trajectory equations for individual particles, using the turbulent instantaneous fluid velocity $u'$, along the particle path during the integration. By computing the trajectory in this manner for a sufficient number of representative particles, which was set by user input, the random effects of turbulence on the particle dispersion was accounted for. The time scale over which a particle interacted with the randomly sampled velocity field was calculated by considering two possible scenarios: (1) the particle moved sufficiently slowly relative to the fluid phase to remain within the eddy during the lifetime of the eddy, or (2) the relative or slip velocity between the fluid and particle was sufficiently large to allow it to traverse across and leave the eddy after a crossing time. The interaction time scale will therefore be the minimum of the eddy lifetime and the crossing time (Tang & Guo, 2011).

With the Reynolds-averaged Navier–Stokes (RANS) models (k-ε, k-ω and RSM), the effect of turbulence on particle trajectory was simulated with the “turbulent dispersion” model. A fluctuation velocity vector is added the time-averaged fluid velocity to simulate the instantaneous fluid velocity at a location of interest. With the isotropic RANS models such as the k-ε and k-ω models, the fluctuation velocity vector is created using turbulence kinetic energy and a random vector with zero mean and unity variance. With the anisotropic RSM turbulence model, the fluctuation velocity is obtained from the anisotropic turbulence properties as part of the flow field solution (Tang & Guo, 2011). To complete the simulation of a particle trajectory, an instantaneous fluid velocity is simulated for every mesh unit where the particle is found. From each particle injection point, a particle is injected 100 times (100 “parcels” in STAR-CCM+ jargon), and 100 different, turbulence-affected particle trajectories were simulated. Particles to be tracked are “injected” at injection points on the inlet surface of the computation domain. In all, for each simulation a total of approximately $10^5$ parcels (particle trajectories) were tracked.

With LES, the turbulence effect on particle trajectory was simulated without the “turbulent dispersion” model. Instead, the effect of turbulence on particle trajectory was simulated through the use of flow field solutions at multiple consecutive time points. For each particle injection point, a particle trajectory was simulated using the flow field solution at a particular instant (by using the “solver frozen” option in STAR-CCM+); then from the same particle injection point, another particle trajectory was simulated using flow field solution at the next instant in LES simulation. This was repeated 100 times, so that for each injection time point, 100 particle trajectories were simulated; the variation of the particle trajectory originated from the same injection point would reflect a pseudo turbulence effect. The LES time step (1 μs or 5 μs) was chosen such that it was much smaller than the Lagrangian time scale of the turbulent flow (approx. 100 μs at Re = 50,000). It should be noted that the “turbulent dispersion” model could also be activated in conjunction with the LES model. However, a test showed that including the turbulent dispersion model had no significant effect on the simulated deposition results, and including turbulent deposition significantly increased the computation time. Therefore, the
Methods of post-processing

(1) Calculation of penetration and dimensionless deposition velocity

Similar to the experimental approach used by Liu and Agarwal (1974), particle deposition was quantified excluding locations near the entrance and the exit of the pipe flow. For that purpose, two plane sections as “derived parts” were created in the CFD control volume, to be used for particle counting and for calculating the penetration for the pipe section in between. These two plane sections were perpendicular to the direction of the flow, at a distance of 127.5 mm and 637.5 mm from the inlet, respectively.

The simulated aerosol penetration, defined as the ratio of the nominal particle mass flow rate at the exit of a pipe flow to that at the entrance, was calculated as:

\[ P = \frac{n_{637.5}}{n_{127.5}} \]  

where \( n_{127.5} \) and \( n_{637.5} \) are the nominal particle mass flow rate at plane sections 127.5 mm and 637.5 mm from the inlet of the computation domain, respectively.

With the penetration known, the deposition velocity can be calculated with the following equation Sehmel (1970):

\[ V_{dep} = \frac{Q}{\pi DL \ln(1/P)} \]  

where \( Q \) is the volumetric flow rate through the pipe, \( D \) is the inner diameter of pipe, \( L \) is the length of the pipe and \( P \) is the aerosol penetration through the pipe section. Then the dimensionless particle deposition velocity can be calculated using Equation (5), where \( u_* \) is the friction velocity defined in Equation (3):

The deposition velocity obtained from the CFD simulations were quantitatively compared with the experimental results. For each flow condition, the relative deviation of the simulated dimensionless deposition velocity from the experimental results was quantified as:

\[ e_r = \exp \left[ \left( \frac{\sum_{i=1}^{N} (\ln V_{exp}^+ - \ln V_{sim}^+)^2}{N - 1} \right)^{0.5} \right] \]  

where \( N \) represents the number of the comparison pairs. When a simulated condition was not available from the experiments, interpolation was carried out to generate an “experimental” \( V_{exp}^+ \) to be compared with the simulated \( V_{sim}^+ \).

(2) Determination of the particle responsiveness factor

A new turbulent deposition parameter – the particle responsiveness factor, \( \alpha \), is defined as the ratio of the wall-normal gradient of the mean square particle velocity fluctuation to the wall-normal gradient of the mean square fluid velocity fluctuation:

\[ \alpha = \frac{\frac{d}{dy} \left( \bar{V}_{py}^2 \right)_w}{\frac{d}{dy} \left( \bar{V}_{fw}^2 \right)_w} \]  

In order to obtain the value of \( \alpha \) from the CFD simulation results, substituting Equation (13) into Equation (6), and replacing the derivative with an expression based on finite difference, and noting \( F_y = 0 \) since these forces are neglected, it yields the following equation, expressed in terms of the quantities at the wall and at the wall-adjacent cell centroids:

\[ \bar{V}_{py,w} \left( \bar{V}_{py,1} - \bar{V}_{py,w} \right) + \bar{V}_{fw,w} \approx -\alpha \frac{d}{dy} \left( \bar{V}_{fw}^2 \right)_w \]  

where \( \bar{V}_{py,w} \) is the particle convective velocity in wall-normal direction at the wall, i.e., the particle deposition velocity that may be obtained from the CFD simulation results using Equation (11); \( \bar{V}_{py,1} \) is the particle convective velocity in the wall-normal direction at the wall-adjacent cell centroid in CFD simulation, which could be obtained from the particle convective flux through a user-defined cylinder section in STAR-CCM+ through the wall-adjacent cell centroids. \( y_1 \) is the distance from the wall-adjacent cell centroid to the pipe wall.

The gradient term on the right-hand side of Equation (14) was obtained from the flow field simulation, to be described below; the two particle convective velocity quantities on the left-hand side were obtained from Lagrangian particle tracking results and Equation (11). Note that in Equation (14), the particle relaxation time \( \tau \) replaces the particle inertial relaxation time \( \tau_i \) which was defined in Equation (7). This approximation shall not introduce significant error for the particle size range involved in this study. (For a 20-micrometer particle, the calculated terminal velocity in air only differs by 0.2% using either \( \tau \) or \( \tau_i \), at a 10-g gravitational acceleration (Hinds, 1999).

To provide references for the CFD-based results to compare against, empirical equations were also used to calculate the particle responsiveness factor. Using the finite difference method, the ratio of \( \frac{d}{dy} \left( \bar{V}_{py}^2 \right)_w \) to \( \frac{d}{dy} \left( \bar{V}_{fw}^2 \right)_w \) was approximated with the ratio of \( \bar{V}_{py}^2 \) to \( \bar{V}_{fw}^2 \) at the wall-adjacent cell centroid, with the assumption that velocity fluctuation would be zero at \( y = 0 \). Thus, the particle responsiveness factor at the wall-adjacent cell centroid may be calculated with an empirical equation (Binder & Hanratty, 1991). The empirical equation was derived based on the measured mean-square particle displacement over the pipe cross section with time, and is valid when the relative velocity between the particle (\( p \)) and the fluid (\( f \)) is small compared to the \( rms \) fluctuation velocity of the fluid.
\((u_f - u_p)/(u^*_{f,p})^{0.5} < 0.5\):

\[
\frac{\nu_{p,f,1}^2}{\nu_f^2} = \frac{1}{1 + 0.7(\tau/\tau_L)}
\]

where \(\tau_{L,1}\) is the Lagrangian time scale of fluid turbulence at the wall-adjacent cell centroid, which is calculated as (Johansen, 1991):

\[
\tau_{L,1} = \frac{v_{t,1}}{\nu_f}
\]

where \(v_{t,1}\) is the fluid turbulent viscosity at the wall-adjacent cell centroid, which is calculated as follows (Davies, 1966):

\[
v_{t,1} = y_{+}^{(4-\gamma_{+0.88})} \left[ \frac{2.5 \times 10^7}{Re} \right]^{-\gamma_{+}/(400+\gamma_{+})} \times 10^{-3} \nu
\]

where the \(y_{+}\) is evaluated at the wall-adjacent cell centroid; \(\nu\) is the kinematic viscosity of the fluid.

(3) Determination of \(\frac{d}{dy}(\frac{\nu_f^2}{\nu_f^2})_w\)

To obtain the wall-normal gradient of the wall-normal mean square fluid velocity fluctuation, \(\frac{d}{dy}(\frac{\nu_f^2}{\nu_f^2})_w\), within the STAR-CCM + framework, a “line derived part” was created, so that the line was in the radial direction as well as parallel to the \(y\) axis, and \(\frac{\nu_f^2}{\nu_f^2}\) on this line was sampled to obtain \(\frac{d}{dy}(\frac{\nu_f^2}{\nu_f^2})_w\) by finite difference. For simplicity of expression, we define:

\[
K = (\frac{\nu_f^2}{\nu_f^2})^2
\]

With the RANS models, the value of \(\frac{\nu_f^2}{\nu_f^2}\) was obtained directly from the flow field simulation; with the LES model, the value of \(\frac{\nu_f^2}{\nu_f^2}\) was obtained by taking the mean square of instantaneous velocity of 5000–10,000 consecutive time steps. Then, \(\frac{d}{dy}(\frac{\nu_f^2}{\nu_f^2})_w\) was obtained using the following equation:

\[
\frac{d}{dy}(\frac{\nu_f^2}{\nu_f^2})_w = \left( \frac{\partial K}{\partial y} \right)_{w} \approx \frac{K_1}{y_{1}}
\]

and a dimensionless form of the quantity was obtained by:

\[
\left( \frac{\partial K}{\partial y} \right)_{w+} = \frac{K_1/u^*_{f}^2}{y_{1}(\frac{u^*_{f}}{u_s})}
\]

where \(K_1\) is the value of \(\frac{\nu_f^2}{\nu_f^2}\) at the wall-adjacent cell centroid, \(u_s\) is the friction velocity of turbulent flow, and \(y_{1}\) is the distance from the wall-adjacent cell centroid to the pipe wall.

Results and discussion

Turbulence model, mesh resolution, and wall treatment all had significant effects on the accuracy of the CFD simulation of turbulent deposition. LES and RSM produced the most accurate results, when using the highest mesh resolution and the all-\(y_{+}\) wall treatment.

Effect of turbulence model

The results with different turbulence models are shown in Figure 2, with a 5-μm thickness for the first prism layer (corresponding to a \(y_{+}\) value of 0.25 at \(Re = 10,000\), and 1 at \(Re = 50,000\)). The experimental results of Liu and Agarwal (1974) and the 2-D RSM simulation result from Parker and Foat (2008) are also shown in these figures. As shown in Figure 2, the CFD simulation results deviated from experimental data significantly when the isotropic turbulence models (k-\(\varepsilon\), k-\(\omega\)) were used; while the LES and RSM simulations had the highest accuracy based on the relative deviation \(e_r\) in Equation (12). Also, the LES (with 1 \(\mu s\) of time step length) and RSM results obtained in this study were more accurate than the 2-D simulation results reported previously (Parker & Foat, 2008). Note that there are significant deviations at small particle sizes (\(\tau_{+} \approx 0.1\)), probably because the small particles’ relaxation time became close to the eddy lifetime or the LES time step, which will be discussed in later sections.

Simulations with RSM and LES turbulence models yielded similar levels of accuracy in terms of particle deposition velocity. The computational cost of LES is high – several weeks for flow field simulation and particle tracking, on a desktop computer with a 2.8 GHz processor, 8GB RAM running 8 parallel processes. Therefore, RSM – only a few days of computation time to produce the flow field and particle tracking results – should probably be the choice of turbulence model for most practical turbulent deposition simulations.

Normalized root mean square wall-normal fluid velocity fluctuation

Figure 3 shows the radial distribution of the dimensionless wall-normal turbulent stress \(u'_{w}\), i.e., the root mean square wall normal fluid velocity fluctuation normalized by the friction velocity \(u'_f = \sqrt{\nu_f^2/\nu_s}\) at half pipe length (0.51 m). As can be seen in the figure, the RANS models and the LES model all overpredicted the wall-normal turbulent stress. However, the results from LES model and the RSM model were the closest to the experimental results. The two isotropic RANS models (k-\(\varepsilon\) and k-\(\omega\)) produced steeper wall-normal turbulent stress gradient than the RSM and the LES models. The RSM results in this study had some distinct differences from the RSM results reported by Parker and Foat (2008), apparently due to the differences in CFD codes and meshing approaches.

For particles involved in this study, turbophoresis is a main driving force for turbulent deposition. Therefore accuracy of the turbulent deposition results strongly depends on the accuracy of the near-wall turbulence gradient. This explains why, among the different turbulence models, the LES and RSM models produced the most accurate deposition velocity estimates (Figure 2).
Effects of near-wall mesh resolution and wall treatment

As shown in Figure 4, the accuracy of the turbulent deposition simulation was dependent on the near-wall mesh resolution. All simulations shown in Figure 4 were with the RSM model and the all-\(y_+\) wall treatment. Figure 4 shows that increasing the wall-adjacent cell size (increasing \(y_+\) value) resulted in overprediction of deposition (the core region mesh size remains the same); only when the

![Figure 2](image)

**Figure 2.** Dimensionless deposition velocity as a function of dimensionless particle relaxation time, CFD-based results compared to the experimental data; all flow conditions included. (For mesh condition where \(y_+ = 0.25\) at \(Re = 10,000\), and \(y_+ = 1\) at \(Re = 50,000\). Fifteen prism layers were used in both Re value cases)

![Figure 3](image)

**Figure 3.** Radial distribution of normalized root mean square wall-normal fluid velocity fluctuation \(\sqrt{\overline{V'^2}}/u_*\) at half pipe length, each data set containing two Reynolds number cases. The RSM results from Parker and Foat (2008) and the experimental data from Durst and Jovanovic (1995) are also plotted.
wall-adjacent cell $y_+$ values were sufficiently low (around unity), were the simulated deposition velocities in good agreement with experiments.

RSM simulation results using two types of wall treatment—high-$y_+$ wall treatment and all-$y_+$ wall treatment—are shown in Figure 5. Using the high-$y_+$ wall treatment resulted in overprediction of particle deposition.

According to the results shown in Figures 4 and 5, both mesh resolution and wall treatment had significant effects on the simulated particle deposition velocity.

The effects of wall-adjacent cell size and number of prism layers observed in this study are similar to those reported for 2-D CFD simulations (Parker & Foat, 2008). Namely, the wall-adjacent cells should be sufficiently small such that the $y_+$ value is on the order of unity, and the number of prism layers should be sufficiently large to cover the near-wall region, where steep gradient of turbulent velocity fluctuation exists.

A sufficiently thin wall prism layer, a sufficient number of prism layers, and properly resolving the near-wall flow are all necessary conditions for accurately resolving the near-wall turbulence. If any of these conditions is not satisfied, the turbulence gradient $\frac{d}{dy}(\overline{V_2^2 y})_w$ will be over-predicted, and so will the particle deposition velocity, as seen in Table 1. The effects of turbulence model, mesh resolution and wall treatment on the accuracy of turbulent deposition simulation observed in this study are similar to those observed in 2-D CFD simulations (Parker & Foat, 2008). This suggests that similar criteria (e.g., near-wall mesh resolution, wall treatment) may be applied to both 3-D and 2-D CFD simulations of turbulent deposition, in order to achieve accurate results. Except for lacking fluid motion in the third dimension, the 2-D RANS models describe turbulent flow the same way as their 3-D counterparts do. Likewise, the EIM model describes particle-eddy interaction the same way in either 2-D or 3-D simulations, except for the different number of spatial dimensions. In other words, the 2-D simulations and 3-D simulations have no fundamental difference in their description of the physics of fluid and physics of particle transport. Therefore, the fact that similar criteria are applicable to both 3-D and 2-D simulations of turbulent deposition in pipe flows is not surprising. From a time-averaged point of view, flow in a circular-cross-section straight pipe is indeed a 2-D flow. Thus it is appropriate to use a 2-D approach to simulate turbulent deposition in such straight pipe flows. However, a 3-D approach must be used for turbulent deposition in true three-dimensional problems encountered in engineering applications, and it is nontrivial to test the 3-D approach in a pipe flow first before implementing it in true three-dimensional problems.

Table 1. CFD-simulated turbulence gradient and particle deposition velocity results with various near-wall mesh settings (RSM model, all $y_+$ wall treatment unless otherwise noted, Re = 10,000), where $K_+ = K/u'_2$.

**Effect of LES time step**

The LES time step was selected to be 1 μs and 5 μs in the present study, so that it was much smaller than the Lagrangian time scale of the turbulent flow (approx. 100 μs at Re = 50,000), when simulating the frozen turbulent flow field at each time step (Johansen, 1991). The two sets of LES results using different time step lengths are shown in Figure 6. Judging by the relative deviation $e_r$, the simulation with the 1-μs time step was more accurate. The deviation of the simulation results from the experimental results was most pronounced for the smallest particle size.

With the LES model, accurately predicting turbulent deposition for small particles is apparently dependent on the ability to resolve the small eddies. Only when the time step is sufficiently small would an LES simulation be able to produce the shortest-lived eddies permitted by a given mesh. For example, when a time step of 10 μs is used, an LES simulation will not produce any eddies that have a lifetime of 1 μs. Intuitively, small
eddie. Only eddies on the edge of the wall can be turbulent, because large particles are less likely to be attracted to small eddies. If particles are attracted to turbulent eddies in the bulk flow, the rate of deposition will be lower. Therefore, if an LES simulation fails to produce eddies that are of significance to certain particle size, it will overpredict the deposition rate for that particle size. The results from this study seem to suggest that the LES time step should be smaller than the particle relaxation time, in order for the turbulent deposition of that particle size to be accurately simulated.

**The particle responsiveness factor**

As shown in Figure 7, the particle responsiveness factor, obtained from CFD simulations, increases as the particle size decreases, and eventually approaches unity; the results agree well with results obtained from empirical
Figure 7. The particle responsiveness parameter $\alpha$ as a function of particle relaxation time $\tau$ for CFD simulation in both Re cases; multiple data points at a given $\tau$ value correspond to multiple turbulence models.

equations (Binder & Hanratty, 1991; Vames & Hanratty, 1988). Note that the relationship between $\alpha$ and $\tau$ appears to depend on the flow Reynolds number; for the same $\tau$ value, $\alpha$ is smaller at higher Re. This suggests that in a higher Reynolds number flow, there exists greater slip between the particle and the fluid. This may be explained by the particles’ inability to follow the higher frequency fluid velocity fluctuation in higher Reynolds number flows (Miller & Dimotakis, 1996; Shang & Xia, 2001). The simulated responsiveness factor had a more significant deviation from the empirical results for smaller particles (e.g., $\tau < 10^{-5}$ s). This was consistent with the fact that the simulated $V_\tau$ deviated from experimental results farther for smaller particles.

Efforts to relate particle motion statistics to fluid motion statistics may also be found in previous studies. Uijttewaal and Oliemans (1996) compare particle root-mean-square (rms) velocity in the radial direction with the fluid rms velocity. The deviation between the fluid and particle rms velocities is found to be dependent on $\tau_+$ as well as on radial location. Wang and James (1999) give results of the particle normal rms velocity and the fluid normal rms velocity for $\tau_+ = 14.3$ and $\tau_+ = 1.1$. Notably, for $\tau_+ = 1.1$ the particle normal rms velocity and the fluid rms velocity curves show significant deviation at the wall. For $\tau_+ = 14.3$, the deviation between fluid rms velocity and particle rms velocity is strongly dependent on the radial location. Wang and Squires (1996) study the correlation coefficient of the wall-normal particle velocity with the wall-normal fluid velocity. It is found that the correlation coefficient decreases with increasing $\tau_+$, but it appears insensitive to the radial location in the flow. The particle responsiveness factor introduced in this study is derived from a Eulerian formulation describing turbulent deposition (Guha, 2008), and is compared against empirical relations obtained experimentally (Vames & Hanratty, 1988). The previous studies do not have such characteristics.

The results in this study suggest that the accuracy of turbulent deposition simulation is critically dependent on the accuracy of the near-wall turbulence simulation. Over-predicting the gradient of the wall-normal fluid velocity fluctuations in the near-wall region leads to over estimating the particle deposition velocity. However, it should be noted that all simulations resulted in similar results of particle responsiveness factor, which agreed well with results based on an empirical equation. In other words, the Lagrangian scheme in the CFD package is adequate and can produce sufficiently accurate simulation of the particle random motion, as long as the turbulent flow field simulation is sufficiently accurate. This further suggests that the accuracy of the near-wall turbulence simulation is the most critical factor for turbulent deposition simulation.

Table 2 shows the root-mean-square (rms) errors of the particle responsiveness parameter $\alpha$ from CFD simulations as compared to the empirical equation results (Binder & Hanratty, 1991). The particle responsiveness factor obtained from the RSM and the LES models had smaller deviations from the empirical-equation results (rms errors 4%-5%). However, the particle responsiveness factor obtained with the k-$\varepsilon$ and the k-$\omega$ models had rms errors up to approximately 9%. These results suggest that the lower accuracy of turbulent deposition simulation with the
k-ε and the k-ω models may also be attributed to the less accurate particle tracking simulation in these models.

The particle responsiveness factor computed from the CFD simulations is evidently a useful index for assessing the accuracy of the particle tracking scheme in a CFD code. One can always use the simulation output for the particle phase and the fluid phase to obtain the responsiveness factor, even without detailed knowledge of the CFD code. The particle responsiveness factor gives the user of a CFD code the ability to assess its particle tracking scheme on a “performance” basis. This is particularly useful for evaluation of nonopen-source commercial CFD packages.

Conclusions

In this study, 3-D simulations of turbulent aerosol particle deposition were carried out using a commercial CFD model, the results of which were compared with experimental results and 2-D simulations from a previous study. A particle responsiveness factor was introduced, whose value was calculated based on post-processing of the CFD simulation results.

Findings and conclusions from this study are similar to those that have been reported from previous studies, in terms of the effects of turbulence model, grid resolution, wall treatment, and time step. Among RANS models the RSM model has the highest accuracy. Sufficiently small wall-adjacent cells are necessary so that the wall y+ values are on the order of unity. A sufficiently large number of prism layers should be used to resolve near-wall flow field without the use of wall functions. When using LES, sufficiently small time step values are necessary to obtain satisfactory results. For LES simulations to yield similar accuracy as with RSM simulations, the former requires much longer computation time. Thus, the more computationally expensive LES may not be practical for simulating all turbulent deposition problems. Over prediction of turbulent deposition velocity for particles with small dimensionless relaxation times is apparently related to the over prediction of the turbulence intensity gradient in the wall-normal direction.

The particle responsiveness factor, introduced for the first time in this study, appears to be a useful index for evaluating the accuracy of the Lagrangian particle tracking schemes. The particle responsiveness factor results suggest that the poor accuracy of turbulent deposition simulation is also attributable to the poor accuracy of the Lagrangian particle tracking scheme. For CFD models to become useful and robust tools for simulating aerosol transport, it is necessary to have accurate results of near-wall turbulence as well as an accurate particle tracking scheme. Furthermore, simulation of turbulent deposition in more complex geometry will require addition experimental validation. Experimental data of turbulent aerosol deposition in complex geometries are currently unavailable, which may be an important area of future research.

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Nomenclature

| Symbol | Definition |
|--------|------------|
| C_c    | Cunningham slip correction factor |
| C_D    | drag coefficient |
| D      | pipe inner diameter |
| d_p    | particle aerodynamic diameter |
| e_r    | relative deviation of CFD simulation from the experiment, in terms of dimensionless deposition velocity |
| F_y    | net force acting on the particles in the y direction |
| f      | Fanning friction factor |
| g_fy   | velocity gradient tensor |
| K      | an alternative expression for \( \sqrt{\frac{\nu}{\nu_f}} \) |
| K_t    | value of \( \sqrt{\frac{\nu}{\nu_f}} \) at the wall-adjacent cell centroid |
| L      | length of pipe |
| N      | number of the comparison pairs used in the calculation of e_r |
| n      | nominal particle mass flow rate in CFD simulation |
| n_127.5 | nominal particle mass flow rate in CFD simulation, at 127.5 mm from pipe inlet |
| n_637.5 | nominal particle mass flow rate in CFD simulation, at 637.5 mm from pipe inlet |
| P      | penetration of aerosol particles in a pipe flow |
| Q      | volumetric flow rate |
| Re     | Reynolds number |
| Re_s   | slip Reynolds number |
| t      | time |
| U      | average fluid velocity in a cross section |
| u      | velocity (vector) |
| \( \overline{u} \) | time-averaged velocity (vector) |
| u'     | turbulence velocity fluctuation (vector) |
| \( u_f \) | local fluid velocity magnitude |
| u_i    | fluid velocity tensor |
| \( u_p \) | particle velocity magnitude |
| u_f    | friction velocity |
| \( V_{dep} \) | particle deposition velocity |
| V^+    | dimensionless particle deposition velocity |
\[ \nu^+ \] dimensionless particle deposition velocity obtained experimentally

\[ \nu^+_{sim} \] dimensionless particle deposition velocity obtained from CFD simulation

\[ \bar{V} \] particle convective velocity

\[ \nabla \] mean square fluid velocity fluctuation in the y (wall-normal) direction

\[ \nabla^2 \] mean square particle velocity fluctuation in the y (wall-normal) direction

\[ v^+ \] normalized root mean square fluid velocity fluctuation position tensor used in velocity gradient expression

\[ \gamma \] distance from the wall

\[ x_j \] dimensionless distance from the wall

\[ \rho_p \] particle responsiveness factor

\[ \tau \] particle relaxation time

\[ \tau^+ \] dimensionless particle relaxation time

\[ \tau_I \] particle inertial relaxation time

\[ \tau_L \] Lagrangian time scale

\[ \tau_{L,1} \] Lagrangian time scale of fluid turbulence at the wall-adjacent cell centroid

\[ \mu \] dynamic viscosity

\[ \nu \] kinematic viscosity

\[ \nu_t \] fluid turbulent viscosity

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