11 Evaluation of continuous and discrete phase models for simulating submicrometer aerosol transport and deposition

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Abstract

Submicrometer aerosols are widely prevalent throughout the environment. Examples of these aerosols include combustion byproducts, ions from radioactive decay, and respiratory-specific viruses. Predicting the transport and fate of these aerosols is important in a number of applications including large-scale environmental assessments, determining pollutant exposure levels in microenvironments, and evaluating the lung deposition and potential health effects of inhaled particles. Numerical simulations of submicrometer aerosols are challenging due to low deposition efficiencies, the action of concurrent inertial and diffusive transport mechanisms, and stiff equation sets. As with other two-phase flow systems, both continuous and discrete phase models have been used to simulate the transport and deposition of submicrometer aerosols. However, each of these approaches has inherent strengths and weaknesses. In this review, the performance of continuous and discrete phase models is assessed in a series of case studies that focus on submicrometer aerosol transport and deposition in the respiratory tract. The numerical methods considered include a chemical species approach that neglects particle inertia, Lagrangian particle tracking, and a recently proposed drift flux model that utilizes a near-wall analytic solution. The performance of these models is evaluated through comparisons with experimental data sets of deposition in a representative double bifurcation geometry, a realistic model of the upper tracheobronchial region, and a realistic model of the nasal cavity. Comparisons of the mass transport methods considered with experimental data highlight advantages and disadvantages of each approach. These results are intended to provide guidance in selecting appropriate two-phase models for simulating submicrometer aerosol transport and deposition in a variety of applications including exposure analysis, respiratory dosimetry, and respiratory drug delivery.

Keywords: Modeling nanoaerosols, Submicrometer aerosol dynamics, Drift flux model, Lagrangian particle tracking
11.1 Introduction

Fine respiratory aerosols can be characterized as having a particle diameter in the range of approximately 100 nm to 1 \( \mu \)m. Inhalable fine aerosols include diesel exhaust products, environmental and mainstream tobacco smoke, and airborne bioaerosols such as viruses and bacteria. Morawska et al. [1] reported average count median diameters of sample diesel exhaust and environmental tobacco smoke to be 125 and 183 nm, respectively. The particle fraction of diesel exhaust can range from 5 to 500 nm [2]. Bernstein [3] summarized a number of studies and reported a consistent value of cigarette smoke count median diameter of approximately 260 nm surrounded by a wide distribution of values ranging from 18 nm to 1.6 \( \mu \)m. Respiratory-specific viruses such as Avian flu and SARS typically range from 20 to 200 nm [4].

Fine aerosols deposit in the respiratory tract at a reduced rate in comparison with smaller ultrafine (<100 nm) and larger coarse (>1 \( \mu \)m) aerosols. This reduction in deposition for fine aerosols is due to a minimum in the net sum of diffusion, sedimentation, and impaction effects [5]. In vivo experiments of whole-lung aerosol deposition in humans indicate a minimum in retention for fine aerosols with a diameter of approximately 400 nm [6–8]. For environmental tobacco smoke and diesel exhaust, the in vivo deposition study of Morawska et al. [1] reported deposition fractions of 36 and 30\%, respectively. While deposition rates are typically low for fine respiratory aerosols, environmental pollutants within this size range are often carcinogenic [9] and inflammatory [10]. As a result, understanding the transport and deposition characteristics of fine respiratory aerosols is critical in order to make accurate toxicology risk assessments, to establish appropriate environmental standards, and to determine safe exposure limits.

Localized accumulations of particles have been widely observed at branching sites in bifurcating respiratory geometries. These focal depositions, or hot spots, are often most pronounced for coarse aerosols due to inertial driven impaction [11–17]. However, significant increases in local deposition have also been observed for dilute submicrometer respiratory aerosols and vapors [17,18–21]. The quantity of particles depositing within a specific localized area will affect the transport of particles and chemical species (CS) across the mucus barrier and ultimately the cellular-level dose received [18]. As a result, evaluations of localized deposition values are needed to better predict cellular-level dose and response [22].

One advantage of computational fluid dynamics (CFD) predictions compared with in vivo and in vitro studies is that modeling results can readily determine localized deposition characteristics in three dimensions. However, due to numerical challenges only few computational studies have quantified the local deposition of fine respiratory aerosols. Zhang et al. [17] compared regional and local depositions of coarse and ultrafine particles, but fine aerosols were not considered. Longest and Oldham [23] modeled the effect of an upstream aerosol delivery system on the deposition of 1 \( \mu \)m aerosols in a double bifurcation geometry. Robinson et al. [24] considered the total deposition of fine respiratory aerosols in a model of...
respiratory generations G3–G8. Longest and Oldham [25] were the first to compare CFD-predicted local depositions of fine aerosols with in vitro data.

Numerical models for simulating particle transport and deposition typically employ either a Eulerian–Lagrangian [18,24,26] or a Eulerian–Eulerian [17,21,27,28] approach for submicrometer aerosol transport and deposition. The Eulerian model that is typically used for respiratory aerosols treats the particle phase as a dilute CS in a multicomponent mixture. This approach neglects particle inertia and only considers deposition due to diffusional effects. However, Longest and Xi [20] illustrated a significant influence of inertia on the regional and local deposition of fine and ultrafine aerosols. In contrast to the CS Eulerian model, the Lagrangian approach tracks individual particles within the flow field and can account for a variety of forces on the particle including inertia, diffusion, gravity effects, and near-wall interactions [29]. Disadvantages of the Lagrangian model include an excessively large number of particles required to establish convergent local deposition profiles and a stiff equation set for fine and ultrafine particles [30]. In the study of Longest and Oldham [23], a Lagrangian model was used to match the overall in vitro deposition rate of 1 µm particles in a double bifurcation geometry; however, the model was not able to match the local deposition characteristics.

In contrast to the CS Eulerian model that is typically applied to ultrafine and fine respiratory aerosols, other continuous field two-phase flow methods are available [31,32]. Respiratory aerosols are typically dilute, such that constant flow field properties can be assumed. However, finite particle inertia has been shown to strongly affect the deposition of fine and ultrafine particles [20]. Of the available two-phase methods, the drift flux (DF) model is an effective approach that can be applied to dilute systems with low Stokes numbers Stk and can account for finite particle forces [33]. Wang and Lai [34] applied a DF model to the deposition of ultrafine through coarse respiratory aerosols to account for gravity and electrostatic effects. However, no previous studies have considered a DF model to approximate the inertia of respiratory aerosols. A potential problem with the DF model applied to fine aerosols is the estimation of particle inertia in the near-wall region.

This chapter will discuss (i) the effect of inertia on the deposition of submicrometer particles and the appropriate bounds for the application of a CS Eulerian model; (ii) development of a new drift flux model that effectively takes into account finite particle inertia; and (iii) evaluation of this new drift flux velocity correction (DF-VC) model by comparisons with experimental data and other model predictions in human respiratory airways. Direct comparisons between numerical and experimental deposition results are made on a regional and highly localized basis. Computational models evaluated include a standard CS mass fraction approximation, Lagrangian particle tracking, and the DF approach to account for finite particle inertia. The airway geometries considered in this study include a idealized bifurcation model, a cast-based tracheobronchial (TB) geometry, and an in vivo scan-based nasal cavity model. Agreement between computational and experimental results will help to establish an effective approach for simulating fine respiratory aerosol deposition where both inertial and diffusional effects may be significant transport mechanisms.
11.2 Models of Airflow and Submicrometer Particle Transport

Flow fields in the respiratory tract are typically assumed to be isothermal and incompressible. Depending on activity conditions, the flow regime under normal breathing can be laminar, transitional, or fully turbulent. Turbulence models have different levels of complexity and include direct numerical simulation (DNS), large eddy simulation (LES), the Reynolds stress model (RSM), and the Reynolds-averaged Navier–Stokes (RANS) two-equation approach. Selection of an appropriate model for the flow of interest mainly depends on the desired accuracy and the available computational resources. DNS is the most accurate approach and resolves turbulent eddies at all scales, but it also requires the most computational resources. Large eddy simulations resolve large-scale energy-containing eddies, and the RSM approach captures the anisotropic turbulence, which is significant near the wall. Even though the lower-order RANS two-equation models cannot account for turbulence anisotropy, these models are still often shown to adequately capture the main features of the flow, provided a very fine mesh is employed in the near-wall boundary region [35]. In this study, the low Reynolds number (LRN) $k - \omega$ two-equation model was selected based on its ability to accurately predict pressure drop, velocity profiles, and shear stress for transitional and turbulent flows [36,37]. This model was demonstrated to accurately predict particle deposition profiles for transitional and turbulent flows in models of the oral airway [38,39], nasal passages [40], and multiple bifurcations [41,42]. Moreover, the LRN $k - \omega$ model was shown to provide an accurate solution for laminar flow as the turbulent viscosity approaches zero [37]. Transport equations governing the turbulent kinetic energy ($k$) and the specific dissipation rate ($\omega$) are provided by Wilcox [37] and were previously reported in Longest and Xi [30].

11.2.1 Chemical species model for particle transport

There is an ever-increasing literature base on particle dynamics in turbulent flows, as reviewed by Crowe et al. [43]. Depending on the need to simulate particle inertia and coupling with the continuous phase, Eulerian-based particle transport models can be categorized as CS, DF, or mixture models. In the respiratory system, dilute suspensions of nanoparticles are often treated as a CS with a Eulerian mass transport model. This model often neglects particle inertia and the effects of the particle phase on the flow field, i.e., one-way coupled particle transport. The transport relation governing the convective–diffusive motion of ultrafine aerosols in the absence of particle inertial effects can be written on a mass fraction basis as:

$$\frac{\partial c}{\partial t} + \frac{\partial (u_j c)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ \tilde{D} + \frac{v_T}{Sc_T} \right] \frac{\partial c}{\partial x_j}$$  \hspace{1cm} (1)

In the above equation, $c$ represents the mass fraction of nanoparticles, $\tilde{D}$ is the molecular or Brownian diffusion coefficient, and $Sc_T$ the turbulent Schmidt number.
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taken to be 0.9. Assuming dilute concentrations of spherical particles, the Stokes–Einstein equation was used to determine the diffusion coefficients for various sized particles and can be expressed as:

\[ \widetilde{D} = \frac{k_B T C_c}{3\pi \mu d_p} \]  

(2)

where \( k_B = 1.38 \times 10^{-16} \text{ cm}^2 \text{ g/s} \) is the Boltzmann constant expressed in cgs units. The Cunningham correction factor has been computed using the expression of Allen and Raabe [44]

\[ C_c = 1 + \frac{\lambda}{d_p} \left( 2.34 + 1.05 \exp\left( -0.39 \frac{d_p}{\lambda} \right) \right) \]  

(3)

where \( \lambda \) is the mean free path of air, assumed to be 65 nm. The above expression is reported to be valid for all particle sizes [45]. To approximate particle deposition on the wall, the boundary condition for the Eulerian transport model is assumed to be \( c_{\text{wall}} = 0 \).

11.2.2 Discrete phase model

One-way coupled trajectories of monodisperse ultrafine particles ranging in diameter \( (d_p) \) from 1 to 1,000 nm are often calculated on a Lagrangian basis by integrating an appropriate form of the particle trajectory equation. Aerosols in this size range have very low Stokes numbers \( \text{St}_k = \rho_p d_p^2 C_c U / 18 \mu D \ll 1 \), where \( U \) is the mean fluid velocity and \( D \) a characteristic diameter of the system. Other characteristics of the aerosols considered include a particle density \( \rho_p = 1.00 \text{ g/cm}^3 \), a density ratio \( \alpha = \rho / \rho_p \approx 10^{-3} \), and a particle Reynolds number \( \text{Re}_p = \rho |u - v| d_p / \mu \ll 1 \). The appropriate equations for spherical particle motion under these conditions can be expressed as:

\[ \frac{dv_i}{dt} = \frac{D u_i}{\tau_p C_c} + \frac{f}{\tau_p C_c} (u_i - v_i) + f_{i, \text{Brownian}} \quad \text{and} \quad \frac{dx_i}{dt} = v_i(t) \]  

(4a and 4b)

In the above equations, \( v_i \) and \( u_i \) are the components of the particle and local fluid velocity, respectively. The characteristic time required for particles to respond to changes in the flow field, or the momentum response time, is \( \tau_p = C_c \rho_p d_p^2 / 18 \mu \). The pressure gradient or acceleration term is often neglected for aerosols due to small values of the density ratio. However, it has been retrained here to emphasize the significance of fluid element acceleration in biofluid flows [29]. The drag factor \( f \), which represents the ratio of the drag coefficient \( C_D \) to Stokes drag, is assumed to be one for submicrometer aerosols. The effect of Brownian motion on the particle trajectories is included as a separate force per unit mass term at each time-step. The amplitude of the Brownian force is of the form [46]

\[ f_{i, \text{Brownian}} = \frac{\pi \rho_p}{\Delta t} \]  

(5)
where $\xi_i$ is a zero mean variant from a Gaussian probability density function, $S_o$ a spectral intensity function directly related to the diffusion coefficient, and $\Delta t$ the time-step for particle integration. The influence of anisotropic fluctuations in the near-wall region is considered by implementing an anisotropic turbulence model proposed by Matida et al. [47], which is described as:

$$u'_n = f_v \xi \sqrt{2k/3} \quad \text{and} \quad f_v = 1 - \exp(-0.002y^+) \quad (6)$$

In this equation, $\xi$ is a random number generated from a Gaussian probability density function and $f_v$ a damping function component normal to the wall for values of $y^+$ less than approximately 40.

### 11.2.3 Deposition factors

For Lagrangian tracking, the deposition efficiency (DE) is defined as the ratio of particles depositing within a region to the particles entering that region. For the Eulerian model, the mass deposition rate on a wall can be expressed as

$$\dot{m}_{w,i} = \sum_{j=1}^{N} -\rho_m A_j \left( \frac{\dot{D}}{Sc} + \frac{v_T}{Sc} \right) \left. \frac{\partial c}{\partial n} \right|_{w,j} \quad (7)$$

where the summation is performed over region of interest $i$, and $n$ is the wall-normal coordinate pointing out of the geometry. Localized deposition can be presented in terms of a deposition enhancement factor (DEF), which quantifies local deposition as a fraction of the total or regional DE. A DEF, similar to the enhancement factor suggested by Balashazy et al. [11], for local region $j$ can be defined as

$$\text{DEF}_j = \frac{\text{DE}_j/A_j}{\sum_{j=1}^{N} \text{DE}_j/A_j} \quad (8)$$

where the summation is performed over the region of interest, i.e., the upper airway geometries. For the Lagrangian model, the local area $A_j$ is assumed to be a region with a diameter of 500 µm, or approximately 50 lung epithelial cells in length [48]. The definition of the DEF is for a pre-specified constant area at each sampling location. Sampling locations are taken to be nodal points. Constant areas are then assessed around each nodal point and allowed to overlap if necessary.

### 11.2.4 Numerical methods

To solve the governing mass and momentum conservation equations in each of the cases considered, the CFD package Fluent 6 was employed. User-supplied Fortran and C programs were implemented for the calculation of initial particle profiles, wall mass flow rates, Brownian force [30], anisotropic turbulence effect [47,49],...
and near-wall velocity interpolation [30]. All transport equations were discretized to be at least second order accurate in space. A segregated implicit solver was employed to evaluate the resulting linear system of equations. This solver uses the Gauss–Seidel method in conjunction with an algebraic multigrid approach to solve the linearized equations. The SIMPLEC algorithm was employed to evaluate pressure–velocity coupling. Convergence of the flow field solution was assumed when the normalized global mass residuals fell below $10^{-5}$ and the residual–iteration curves for all flow parameters become asymptotic.

11.3 Evaluation of Inertial Effects on Submicrometer Aerosols

A direct comparison between the Eulerian and Lagrangian transport model results can be visualized in a branching respiratory geometry by snapshots of particle locations at two selected times during a washout phase with a tracheal flow rate of 30 L/min (Figure 11.1). The initial velocity profile was parabolic resulting in a near-wall region of low flow beginning at the inlet. For each model, 5 nm particles were initially released from an inlet plane for 0.003 seconds. The simulation was then continued over time to illustrate the washout of the remaining particle fraction. For the Eulerian simulation at $t = 0.005$ seconds, a high concentration region is observed to interact with the first carina and inner walls of the daughter branches (Figure 11.1a). However, these elevated concentrations have been eliminated from the first carina by time $t = 0.015$ seconds due to the high velocities in this region (Figure 11.1b). Moderately elevated concentrations of mass fraction are observed near the second carinas at $t = 0.015$ seconds (Figure 11.1b). As the simulation continues from $t = 0.005$ to 0.015 seconds, washout of the mass fraction is observed in regions of high flow, whereas regions of low flow are dominated by mixing.

Snapshots of Lagrangian particles appear similar to the Eulerian mass transport model over time (Figure 11.1c and d). For time 0.005 seconds, a region of high concentration is again observed to interact with the first carinal ridge. However, the Lagrangian particles simulated have not progressed as far as the minimum contour level considered for the Eulerian flow (Figure 11.1a vs. c). This may be due to the discrete nature of the Lagrangian particles and the relatively small number of particles considered for this illustration. Approximately 2,000 particles were tracked for visualization. However, the Lagrangian model also directly accounts for the molecular slip correction and Taylor diffusion. At time 0.015 seconds, the Eulerian and Lagrangian models again appear similar (Figure 11.1b vs. d). It is noted that the Eulerian model is presented for a mid-plane slice, whereas the Lagrangian model must be presented in terms of particles in the 3-D field. Therefore, the mid-plane view of the Eulerian model reveals only a thin near-wall region of elevated concentration in G3 at time 0.015 seconds (Figure 11.1b). In contrast, this thin near-wall concentration layer of slow-moving particles is observed to occupy a majority of the third generation based on the 3-D view through the geometry for the Lagrangian result (Figure 11.1d).
Figure 11.1. Comparison of Eulerian species mass fraction (a and b) and Lagrangian particle distributions (c and d) at various times for an inhalation flow rate of 30 L/min in the upper airway model. A constant concentration of 5 nm particles was released at the inlet plane for the first 0.003 seconds of the simulation.

Figure 11.2 shows the regional deposition fractions based on both Eulerian and Lagrangian particle tracking models in comparison to experimental and analytical results within an upper airway double bifurcation geometry (generation G3–G5) for a tracheal flow rate of 30 L/min. Predictions of the Eulerian transport model are consistent with the correlation of Cohen and Asgharian [50] as well as the analytic solution of Ingham [27] (Figure 11.2). Based on available empirical data, the correlation of Cohen and Asgharian [50] is valid for particles from 40 to 200 nm and includes a high degree of variability. Over this range, good agreement is observed between the Eulerian and empirical models (Figure 11.2). The particle size and Stokes number for which the Lagrangian particle deposition fraction exceeds Eulerian particle deposition by a difference of 20% has been marked (Figure 11.2). This particle size is considered to be the threshold where impaction plays a significant role in total deposition fraction and will be referred to as the inertial particle diameter. At 30 L/min, the inertial particle diameter is 120 nm and...
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20% variation in Eulerian and Lagrangian simulations (120 nm)

\[ St_3 = 5.0 \times 10^{-5} \]

Particle diameter (nm)

Cohen and Asgharian (1990)
Ingham (1991)
Martonen (1993)
Eulerian simulation
Lagrangian particle
Lagrangian fluid element

Figure 11.2. Branch-averaged deposition fraction in respiratory generations G3–G5 of the upper airway model for an inhalation flow rate of 30 L/min. Good agreement is observed between the simulated results and the empirical correlation of Cohen and Asgharian (1990) from 40 through 200 nm. Separation of Eulerian and Lagrangian simulation results indicates the onset of particle impaction. Particle impaction is observed to become significant for 120 nm particles.

the associated Stokes number for generation G3 is \( 5.0 \times 10^{-5} \). As the flow rate is increased, the minimum particle size where impaction becomes important grows smaller due to increasing flow inertia. The smallest observed inertial particle diameter was 70 nm (\( St = 5.1 \times 10^{-5} \)), which occurred for the highest tracheal flow rate considered, which was 60 L/min.

To ensure accuracy in the particle tracking routine, the deposition fraction of massless Lagrangian fluid elements has also been assessed (Figure 11.2). Fluid elements are assumed to have the density of the continuous fluid, or air, resulting in negligible inertia effects. The diffusion of fluid elements is based on the geometric element diameter and is not influenced by the density. The resulting deposition fraction of Lagrangian fluid elements is observed to be in close agreement with the Eulerian model results for all particle sizes considered (Figure 11.2). Therefore, differences in the Lagrangian and Eulerian solutions may be assumed to represent the effects of finite particle inertia and not numerical errors in the particle tracking routine.

In comparison to regional-averaged values, the effects of particle inertia on localized deposition characteristics were found to be much more dramatic [20,40,42]. As shown by Longest and Xi [20], for the upper airway bifurcation
model, inclusion of particle inertia was found to increase the maximum local microdosimetry factor by one order of magnitude for 40 nm particles at an inhalation flow rate of 30 L/min. The maximum DEF values predicted by the Lagrangian model was 103.9 in contrast to a $\text{DEF}_{\text{max}}$ of 5.7 predicted by the Eulerian CS model [20]. It was also observed that the Lagrangian model did not appear to resolve continuous contours of DEF below values of approximately 5.

From the above observations, it is indicated that particle inertia may be more significant in the regional and local deposition of fine and ultrafine aerosols than previously considered. Therefore, CS Eulerian models of particle transport may significantly underestimate branch-averaged and local deposition values of fine and ultrafine particle deposition. This underestimation was found to be especially significant for localized deposition patterns and microdosimetry estimates. For 40 nm particles, a one order of magnitude increase of the DEF values was observed in Lagrangian estimates in comparison to Eulerian predictions for the upper airway model at an inhalation flow rate of 30 L/min. Furthermore, the particle inertia cannot be ignored for regional deposition calculations with Stokes numbers larger than $5.0 \times 10^{-5}$ in bifurcating airways. As a result, it is necessary to develop an appropriate particle transport model that can effectively resolve continuous contours of deposition and capture the influence of finite particle inertia for submicrometer aerosols in the respiratory tract.

11.4 An Effective Eulerian-Based Model for Simulating Submicrometer Aerosols

The basis of this Eulerian approach is the DF model with a novel extension to better compute wall deposition on a continuous basis. In contrast with the CS model, the DF approach includes particle inertial effects, which are taken into consideration through the convection term [25,33]

$$\frac{\partial c}{\partial t} + \sum_{j} \frac{\partial (v_j c)}{\partial x_j} = \sum_{j} \left( \frac{\nabla}{Sc_T} \right) \frac{\partial c}{\partial x_j}$$

In this equation, $v_j$ is the particle velocity, which is evaluated from the particle slip velocity ($v_{sj}$) as:

$$v_j = v_{sj} + u_j$$

For a continuous field solution, the particle slip velocity can be determined as a function of inertial and gravity forces as [33]

$$v_{sj} = \frac{C_c}{18\mu_c} \frac{d_p^2}{\rho_p - \rho_m} \left[ g_j \frac{\partial u_j}{\partial t} - u_i \frac{\partial u_j}{\partial x_i} \right]$$

where $C_c$ is the Cunningham correction factor, $\rho_p$ and $\rho_m$ are the particle and mixture densities, $d_p$ the particle diameter, and $\mu_c$ the continuous field viscosity.
variables

\[ n - \text{wall normal coordinate} \]
\[ s - \text{distance between CV center and wall} \]
\[ u - \text{fluid velocity} \]
\[ v - \text{particle velocity} \]

subscripts

\[ CV - \text{control volume center} \]
\[ p - \text{particle position} \]

Figure 11.3. Velocity components and notation within a near-wall control volume.

In equation (11a), the first term in brackets is the gravity vector and the next two terms represent the material derivative, which accounts for fluid element acceleration. For the small particles considered in this study (\( \leq 1 \mu m \)), gravity effects are neglected and Stokes flow conditions can be assumed. As a result, equation (11a) can be written in terms of the fluid pressure gradient as [33]:

\[
v_{s_j} = \frac{C_c d_p^2 (\rho_m - \rho_p)}{18 \mu_c} \frac{\partial p}{\partial x_j}
\]  

(11b)

As with the CS model, the DF approach approximates perfect absorption at the wall, i.e., \( c_{\text{wall}} = 0 \). The associated local mass deposition as a result of both diffusional and inertial effects is expressed as:

\[
\dot{m}_{w,l} = -\rho_m A_l \hat{D} \frac{\partial c}{\partial n} \bigg|_{\text{wall}} + \rho_m A_l c v_n \big|_{\text{wall}}
\]  

(12a)

In the above expression, \( v_n \) represents the wall-normal particle velocity scalar

\[
v_n = v_i \hat{n}_i
\]  

(12b)

where \( \hat{n}_i \) is the local wall-normal unit vector pointing out the geometry.

Differences among the two DF approaches considered in this study are based on how the particle velocity at the wall is computed and implemented in the particle deposition expression, equation (12a). Velocity values near the wall on a control volume grid and related nomenclature are indicated in Figure 11.3. For the standard DF model, slip velocities are only available at control volume center locations. As a result, the particle velocity at the wall is approximated as the value at the center of the nearest control volume, i.e.,

\[
v_n \big|_{\text{wall}} = v_{cv,i} \hat{n}_i = v_{cv,n}
\]  

(13)

As indicated in Figure 11.3, the subscript \( CV \) indicates the value at the control volume center and the subscript \( n \) indicates the wall-normal scalar. Based on expected particle deceleration between the control volume center location and the wall...
surface, the standard DF approximation is expected to significantly overestimate particle inertia at the wall and may be mesh dependent.

To improve performance of the standard DF approach, velocity corrections are proposed for particle conditions at the initial point of particle-to-wall contact. Instead of utilizing velocity at the near-wall cell center as with the standard DF model, the particle velocity at the wall is determined based on a subgrid solution of particle motion between the control volume center and wall location. The motivation behind this subgrid solution is that fully resolving near-wall finite particle inertia with a continuous model would require an excessive number of control volumes. Instead, the DF-VC model employs an analytic solution of particle velocity between the near-wall control volume center and the wall (Figure 11.3). It is assumed that the continuous field model approximates particle diffusion within this region. Furthermore, for low particle Reynolds numbers the individual Lagrangian transport terms become linear and separable. Particle inertia between the control volume center and wall surface can then be approximated on a discrete Lagrangian basis as:

$$\frac{dv_{p,n}}{dt} = \frac{1}{\tau_p}(u_{p,n} - v_{p,n})$$ (14)

To formulate an analytic solution of equation (14), the wall-normal fluid velocity is assumed to vary linearly between the control volume center and zero at the wall. The resulting equation for particle position between the near-wall control volume center and the wall as a function of time can be written as

$$\frac{d^2x_p}{dt^2} + \frac{1}{\tau_p} \frac{dx_p}{dt} + \frac{u_{cv,n}}{\tau_p} x_p = \frac{1}{\tau_p} u_{cv,n}$$ (15)

where $u_{cv,n}$ is the fluid velocity at the control volume center location normal to the wall. An analytic solution to equation (15) is possible resulting in wall-normal expressions for particle position

$$x_p(t) = \frac{v_{cv,n} + \lambda_2 s}{\lambda_1 - \lambda_2} e^{\lambda_1 t} - \left( \frac{v_{cv,n} + \lambda_2 s}{\lambda_1 - \lambda_2} + s \right) e^{\lambda_2 t} + s$$ (16a)

and velocity

$$v_{p,n}(t) = \frac{v_{cv,n} + \lambda_2 s}{\lambda_1 - \lambda_2} \lambda_1 e^{\lambda_1 t} - \left( \frac{v_{cv,n} + \lambda_2 s}{\lambda_1 - \lambda_2} + s \right) \lambda_2 e^{\lambda_2 t}$$ (16b)

where

$$\lambda_1 = \frac{1}{2} \left( -\frac{1}{\tau_p} + \sqrt{\left( \frac{1}{\tau_p} \right)^2 - 4 \left( \frac{u_{cv,n}}{\tau_p} \right)} \right)$$ (16c)

$$\lambda_2 = \frac{1}{2} \left( -\frac{1}{\tau_p} - \sqrt{\left( \frac{1}{\tau_p} \right)^2 - 4 \left( \frac{u_{cv,n}}{\tau_p} \right)} \right)$$ (16d)
The time for initial wall contact can be determined from equation (16a). The associated particle velocity at the point of deposition is then calculated using equation (16b) and applied to calculate the local mass deposition in equation (12a).

The expressions for near-wall particle position and velocity presented as equations (16a and b) require the \( \lambda \) coefficients (equations 16c and d), which are roots of the characteristic equation for particle motion, to be real and unique. If these coefficients are complex numbers or repeated roots, then the general solution of near-wall particle motion will have a different form. The occurrence of real and unique values of \( \lambda_1 \) and \( \lambda_2 \) requires that

\[
\left( \frac{1}{\tau_p} \right)^2 > 4 \left( \frac{u_{cv,n}}{s\tau_p} \right)
\]

(17)

The particle response time (\( \tau_p \)) is proportional to the particle diameter squared. Therefore, the condition for real and unique values of \( \lambda_1 \) and \( \lambda_2 \) is more likely to be satisfied for smaller particles. As the particle size increases, the left-hand side (LHS) of the condition decreases rapidly, which increases the probability for complex values of \( \lambda_1 \) and \( \lambda_2 \). Considering submicrometer aerosols, the limiting maximum particle size is 1 \( \mu \)m, which should result in only real and unique values of \( \lambda_1 \) and \( \lambda_2 \), as verified numerically [42].

### 11.5 Evaluation of the DF-VC Model in an Idealized Airway Geometry

In this section, three continuous field models were evaluated based on their ability to capture the inertial effects of submicrometer aerosols by direct comparisons with in vitro experimental data in a idealized bifurcation geometry. The first model considered was the Eulerian CS approximation, which is known to neglect particle inertia [20]. Implementation of this model is intended as a base case to capture purely diffusional effects. The remaining two models were based on a DF approach that accounts for both diffusion and particle inertia effects. Differences in the DF models arise as a result of how the near-wall inertia is approximated, as described in the previous section. The idealized airway bifurcation model was selected here as a test case because it can be mathematically described, which facilitates the generation of identical experimental and computational geometries.

The experimental method for the generation and delivery of submicrometer aerosols was previously described by Oldham et al. [15]. Briefly, a Lovelace-type compressed air nebulizer (In-Tox Products, Albuquerque, NM) was used to generate the fluorescent 400 nm and 1 \( \mu \)m aerosols. As shown in Figure 11.4a, a custom copper enclosure [51] was used to connect the nebulizer with the double bifurcation model. Aerosols were dried and diluted using 5% relative humidity air at an inject rate of 10 times the nebulizer output. The aerosol was discharged to Boltzmann equilibrium by passing through a \(^{85}\)Kr discharger. Aerosols were pulled through the double bifurcation models by use of a vacuum pump. Particles that did not
Figure 11.4. Geometries considered including (a) experimental particle delivery system, and (b) double bifurcation model of respiratory generations G3–G5.

deposit in the models were collected on a 25 mm diameter polycarbonate filter with a 0.1 µm pore size (Nucleopore Corporation, Pleasanton, CA). Local and total depositions of aerosols were determined by microscope-based counting on a grid of 1.4 × 0.95 mm for 1 µm particles and 1 × 0.69 mm for 400 nm particles [25,15]. Fluorescent particle counts in photographic microscope fields were determined using fluorescence microscopy.

Comparisons of experimental and numerical total particle deposition values in the bifurcation geometry for the two particle sizes considered are illustrated in Figure 11.5. For 400 nm particles, the experimental total deposition rate is 0.0054%. The CS model appears to closely match the experimental deposition value with a total deposition prediction of 0.0048%, resulting in a percent difference of 11.1%. In contrast, the standard DF model predicts a deposition rate that is nearly two orders of magnitude higher than the experimental findings. As a result, the standard DF model appears to significantly overpredict the effects of particle inertia. The DF-VC approximation matches the experimental results to a high degree with a total deposition value of 0.00585% and a percent difference 8.3%. As a result, both the CS and DF-VC models appear to provide adequate predictions of total deposition for 400 nm particles. Comparisons of local deposition results with experimental findings will be used to evaluate differences between the CS and DF-VC models.

Experimental deposition results for 1 µm particles indicate a total deposition fraction of 0.01% (Figure 11.5), as reported in Oldham et al. [15]. Due to a lack of particle inertia in the computational model, the CS approach under predicts the total deposition fraction for 1 µm aerosols by one order of magnitude. In contrast, the standard DF model overpredicts the total deposition by one order of magnitude. As with 400 nm particles, predictions of the DF-VC model for 1 µm particles are in close agreement with experimental results. The DF-VC model predicts a total deposition value of 0.0104%, resulting in a difference of 4.0% in comparison with the experiment.
Figure 11.5. Comparison of total deposition fraction as a percentage between experimental results and model predictions for 400 nm and 1 μm particles.

Experimental results of local 400 nm particle depositions on a 1 × 0.69 mm grid are shown in Figure 11.6a as a percentage of total deposited particles [25]. As expected, localized increases in particle deposition are observed at the bifurcations. Deposition contours are in the range of 1 to 5% at the first carinal ridge and 0.1 to 1% at the second. A discontinuous shading pattern is observed in the first daughter branches with contours in the range of 0.01 to 1%. At the second bifurcation, higher contour values appear to extend down the inner branch in comparison with the outer branch. Some asymmetry in the deposition pattern may be due to minor variations in the inlet particle concentration and alignment of the grid field with the experimental model.

Numerical results of local particle deposition for 400 nm aerosols are reported on a two-dimensional grid with element sizes equivalent to the experimental study, i.e., 1 × 0.69 mm (Figure 11.6b–d). For the CS model and 400 nm particles, hot spots of local particle deposition are not observed at the carinal ridges (Figure 11.6b). As a result, the CS model appears to match the experimental total deposition value but displays significant differences from local experimental findings. Moreover, the CS model appears to predict more evenly distributed contours of deposition throughout the physiologically realistic bifurcation (PRB) in comparison with the experimental results. Considering the standard DF model, a significant increase in local particle deposition is observed at the first carinal ridge and a lesser hot spot occurs at the second bifurcation point (Figure 11.6c). However, these hot spots are at a higher contour level than observed in the experiment and surrounded by few deposited particles. The DF-VC model provides the best match to localized experimental results for the deposition of 400 nm particles (Figure 11.6d). Maximum localized particle deposition values at both carinal ridges are predicted to be within the same range as observed experimentally. Specially, the DF-VC model
Figure 11.6. Comparison between experimental and numerically determined contours of local deposition for 400 nm particles expressed as a percentage of total deposition: (a) experimental, (b) CS, (c) DF, and (d) DF-VC models.

Predicts localized deposition at the first and second carinal ridges to be 1 to 5% and 0.1 to 1%, respectively. Furthermore, the DF-VC model predicts elevated contours within the range of 0.1 to 1% extending down the inner branch of G5, as observed experimentally. Similar agreements between model and experimental results were also observed for 1 µm particles [25].

A significant finding from this direct comparison was that the CS and standard DF models did not effectively predict the deposition of fine respiratory aerosols. The CS model has been widely applied in respiratory dynamics systems for particles up to approximately 100 nm [20,21,52,53]. However, only a few available studies have applied a DF model for the simulation of respiratory aerosols [34,54]. No previous study has implemented a DF model to determine the inertial deposition of fine respiratory aerosols. Based on the available two-phase flow literature, the standard DF model should adequately model the deposition of dilute fine respiratory...
aerosols based on diffusional and inertial transport mechanisms [32,33]. However, results of this study indicated a significant overprediction of respiratory aerosol deposition with use of the standard DF formulation. This overestimation was due to significant changes in particle slip velocity between the near-wall control volume center location and conditions at particle-to-wall contact.

11.6 Evaluation of the DF-VC Model in Realistic Airways

In this section, the DF-VC model was extended to transient conditions and was tested in more complex geometries of the respiratory tract for laminar and turbulent flows. Particle transport and deposition were evaluated in a computational replica of the TB geometry and an MRI-based nasal model. Numerical results were compared to existing experimental data in these models. A standard CS model was also considered to evaluate the extent to which the DF-VC model captures the effects of particle inertia. To determine the influence of time effects on particle deposition, steady and transient flow fields were evaluated. These studies are intended to further develop a highly effective method for the simulation of fine respiratory aerosols in realistic models of the upper airway.

11.6.1 Tracheobronchial region

A hollow cast of the human TB tree (Figure 11.7a) utilized by Cohen et al. [55] was digitally replicated in this study to ensure a direct comparison with experimental deposition results. The geometric parameters of the cast were in agreement with population means of a representative average adult male. The original cast used in the study of Cohen et al. [55] was scanned by a multirow-detector helical CT scanner (GE medical systems, Discovery LS) with the following acquisition parameters: 0.7 mm effective slice spacing, 0.65 mm overlap, 1.2 mm pitch, and 512 × 512 pixel resolution. The multislice CT images were then imported into MIMICS (Materialise, Ann Arbor, MI) to convert the raw image data into a set of cross-sectional contours that define the solid geometry. Based on these contours, a surface geometry was manually constructed in Gambit 2.3 (Ansys, Inc.) (Figure 11.7b and c). Some distal branches in the range of generations G5 and G6 were not retained in the digital model due to low resolution. Most of the digital model paths extended from the trachea to generation G4 with some paths extending to generations G5 and G6. Twenty-three outlets and a total of 44 bronchi were retained in the final computational model (Figure 11.7b). The surface geometry was then imported into ANSYS ICEM 10 (Ansys, Inc.) as an IGES file for meshing. To avoid excessive grid elements, some minor smoothing of the geometric surface was necessary.

The left–right asymmetry, which is an important feature of the human lung, was preserved in the TB model. There are three lobes in the right lung and two lobes in the left. As observed in the TB model, the left main bronchus is approximately 2.5 times longer than the right (Figure 11.7b), which is consistent with van Ertbruggen et al. [56]. For conducting airways, the bifurcating pattern is typically asymmetric.
Figure 11.7. Development of a tracheobronchial airway model from a replica cast of the human upper respiratory tract: (a) the hollow cast utilized by Cohen et al. [14] showing the divisions of sub-branch segments. A mechanical larynx was connected to the cast in order to generate cyclic inspiratory flows. (The figure was provided by Dr. Beverly Cohen, NYU School of Medicine.) (b) A surface geometry was constructed based on CT scans of the cast and software packages MIMICS and Gambit. Using ANSYS ICEM 10, the computational mesh was generated and consisted of unstructured tetrahedral control volumes with a very fine near-wall grid of prism elements.

with daughter branches from the same parent often differing both in diameter and length. Additionally, the spatial orientations of the bifurcating branches are quite variable, resulting in a lung architecture that is highly out-of-plane.

A critical feature of the physiologically realistic TB model used in this study is the inclusion of a laryngeal approximation and wedge-shaped glottis, as shown in Figure 11.7b and c. Including a laryngeal approximation provides a better representation of in vivo conditions and is significant in deposition studies with TB casts [57]. Studies by Chan et al. [58], Gurman et al. [59], Martonen et al. [60], and recently Xi et al. [35] have highlighted the significance of the laryngeal jet on downstream deposition in the respiratory tract. The transient breathing conditions of Cohen et al. [55] were approximated as a sinusoidal function with the format

$$Q(t) = Q_{in} [1 - \cos (2\omega t)]; \quad u(t) = u_{mean} [1 - \cos (2\omega t)]$$  \hspace{1cm} (18a and b)

where $\omega$ is the breathing frequency in radians/s.

Compared with the idealized bifurcation model, interesting flow phenomena are observed due to the complex geometry characteristics of the TB model such as the presence of the larynx, left–right asymmetry, and non-coplanar bifurcations. The laryngeal jet that forms at the glottis aperture extends downstream through the
trachea and is skewed toward the right wall (Figure 11.8). Flow reversal occurs in the trachea due to the strong jetting effect. As a result, a large recirculation zone develops near the left tracheal wall, which significantly reduces the cross-sectional area available for expansion of the high-speed flow. Similar results have been reported by Corcoran and Chigier [61]. Using Laser Doppler Velocimetry and fluorescent dye, Corcoran and Chigier [61] also observed a skewed laryngeal jet in the right anterior trachea and a region of reverse flow in the left trachea with a cast model. The skewed jet feature may have physiological implications that facilitate efficient mixing and deeper penetration of inhaled oxygen into the lung. Conversely, higher particle deposition rates are expected on the right tracheal wall and in the right downstream branches due to impaction.

Figure 11.8. Midplane velocity vectors, contours of velocity magnitude, and in-plane streamlines of secondary motion in the tracheobronchial model under steady conditions with an inspiratory flow rate of 34 L/min. The slices are not to scale.
For transient inlet conditions of a mean flow rate of 34 L/min, the Womersley number ($\alpha$) ranges from 4.2 to 0.8 in the conducting airways of G0 to G6, indicating moderate to small unsteady effects. As expected, transient flow patterns are similar to steady state conditions for a major portion of the breathing cycle (i.e., $0.15T$ to $0.85T$), resulting in what can be considered as a quasi-steady system [42]. In contrast, during the transition phase between breathing cycles when the velocity is small, the fluid experiences dramatic changes in both mainstream flow and secondary motion [35,42]. Similarly, Kabilan et al. [62] examined the flow characteristics in a CT-based ovine lung model. Their results suggested that the onset of the transient phase of the flow might be the main cause of vorticity formation, which plays an important role in gas mixing. Li et al. [63] also reported that particle deposition has a strong dependence on individual phases of the transient waveform.

Comparisons of experimental and numerical values of total deposition in the TB model geometry for 40 and 200 nm particles are illustrated in Figure 11.9. The experimental deposition values were reported by Cohen et al. [55] for cyclic breathing with a mean flow rate of 34 L/min and a breathing frequency of 20 breaths per minute. The transient numerical deposition fraction is a cumulative value that includes both the particle-release phase (2nd cycle) and the following washout phase (3rd and 4th cycles). The first cycle is airflow only, without particles, in order to establish the transient flow field within the TB geometry. In the case of 40 nm particles, the experimental total deposition rate is 0.7%. Both the CS and DF-VC models closely match the experimental deposition value under steady conditions with a total deposition prediction of 0.706 and 0.714%, respectively. The marginally higher total deposition value of the DF-VC model indicates a negligible contribution of inertia to total deposition for 40 nm particles. In contrast, both models appear to underestimate the experimental result for transient conditions, resulting in a percent error of $-48.9\%$ for the transient CS model and $-21.1\%$ for the transient DF-VC model.
Experimental cyclic deposition results for 200 nm particles indicate a total deposition fraction of 0.38% (Figure 11.9). Due to a lack of particle inertia, the CS model significantly under predicts the total deposition fraction for 200 nm aerosols, resulting in percent errors of $-52.1\%$ for steady ventilation and $-81.3\%$ for cyclic ventilation. The DF-VC model provides a substantial improvement over the CS approach by incorporating the particle inertia forces in the computational model. As with 40 nm particles, predictions of the DF-VC model for 200 nm particles with steady flow are in close agreement with the experimental results, with a minor underestimation of $-8.4\%$. For cyclic conditions, the DF-VC approach predicts a total deposition of 0.257%, resulting in a difference of $-32.4\%$ in comparison with the experiment. Comparing these two models, differences between the CS predictions and the experimental results are significant for 200 nm particles, indicating a significant contribution from particle inertia. Still, an under prediction of deposition for 200 nm particles is observed with the DF-VC model. As noted before, some distal branches of the TB cast were not included in the numerical model and a static open glottis was employed, which may contribute to this under prediction of the experimental results for both steady and transient inhalation conditions.

Figure 11.10 illustrates the DEF value for the DF-VC model under cyclic conditions with a mean flow rate of 34 L/min. For the DF-VC model, the deposition patterns under steady and cyclic conditions are similar in appearance for 40 and 200 nm particles, respectively. However, more concentrated local deposition values in the larynx and bifurcations are obtained under cyclic conditions compared with steady state. Specifically, the maximum DEF value for 200 nm aerosols with cyclic flow (i.e., 267) is about seven times higher than with the steady condition (i.e., 37),

Figure 11.10. Numerically determined deposition enhancement factors (DEF) in the tracheobronchial airway under transient conditions at a mean flow rate of 34 L/min with the DF-VC model for (a) 40 nm and (b) 200 nm particles.
indicating a dramatic increase of the velocity-dependent inertia effect on particle localization. For the smaller 40 nm particles, the maximum DEF value of approximately 18 for cyclic inhalation is only twice as large as the steady state value of 8.3. As a result, transient conditions have a greater effect on the deposition of a 200 nm aerosol, in comparison with 40 nm particles, due to inertial effects.

Geometric complexity, turbulence, and transient flow are all expected to significantly influence the deposition of aerosols in the respiratory tract \[38,64–66\]. In this context, an extended DF-VC model was evaluated by comparing with experimental results in a complex TB geometry with transient and laminar-to-turbulent flows. Through comparison with the CS model, the DF-VC approach was shown to better capture the expected effects of particle inertia on a total and local basis.

11.6.2 Nasal cavity

The DF-VC model was further tested in a human nasal airway, which was based on MRI scans of a healthy non-smoking 53-year-old male (weight 73 kg and height 173 cm). The procedure for developing the nasal airway geometry and mesh is similar to the approach applied for the TB model in the previous section. As shown in Figure 11.11, the nasal cavity is characterized by narrow, convoluted, and multilayer channels called meatus. This complex passageway generates unique aerodynamics inside the nasal cavity and helps the nose to accomplish its physiological functions. Conversely, reasons for deficient nasal function can often be traced back to abnormal
global and local flow conditions and turbulent phenomena in the nasal passages. In an adult, 18,000 to 20,000 L of air pass through the nose each day. Besides warming and moistening the inhaled ambient air, the nasal cavity also houses olfactory sensory receptors, filters out airborne pollutants, drains excess sinus secretions, and balances pressure between the middle ear and atmosphere.

As in the previous section, two continuous field particle transport models, i.e., CS and DF-VC models, are considered. To highlight the effect of finite particle inertia on deposition localization, a comparison of DEFs predicted using the CS and DF-VC models are shown in Figure 11.12 for 400 nm particles at an inhalation flow rate of 30 L/min. With DEF values plotted on the same scale, the difference between these two models is striking. In contrast to the more uniformly distributed DEF values of the CS model, the deposition with the DF-VC model is significantly more heterogeneous and localized. Specifically, at the anterior junction point (solid circle) between the middle meatus and medial passage where high-speed flow and steep geometry transition occur, the hot spot of the DEF value predicted by the DF-VC model is about five times higher than the CS value. Another expected hot spot is at the superior part of the vestibule (dashed square), which is captured by the DF-VC model. In contrast, the CS model does not indicate this region as having elevated deposition. Additionally, elevated deposition accumulations are also predicted around the rear olfactory region (filled arrow) based on the DF-VC model due to trajectory deviations of large particles from curved streamlines in the main airflow. These elevated localizations may have important implications in chemical sensing applications or nasal drug delivery for neurological disorders where the olfactory region is the targeted deposition site.

The effectiveness of the DF-VC model in capturing inertial and diffusive deposition is further illustrated in Figure 11.13 in terms of deposition within specific sections of the nose. The definition of each section is depicted in Figure 11.11.
and the inhalation conditions are identical to those shown in Figure 11.12 (i.e., $Q_{in} = 30$ L/min and 400 nm particles). The magnitude of the deposition fraction value for each region (except for the nasopharynx) represents the summation of right (lower bar) and left (upper bar) nasal passages. The deposition fraction values for the CS model denote deposition from diffusion only, while the difference between the DF-VC and CS models can be viewed as deposition from inertial impaction. In the vestibule, where the direction of airflow changes by approximately $90^\circ$, significantly enhanced deposition is predicted by the DF-VC model, which is about 6.1 times the CS model estimate for identical conditions. An even more pronounced effect of inertial impaction (i.e., an order of magnitude increase) is found in the nasal valve region where the cross-sectional area is minimal and the airflow passages are narrowest. In this region, the valve-associated stenosis, flow acceleration, and short distances to the walls combine to effectively increase the inertial deposition of particles entrained in the flow. The inertial effect on deposition in the main passage remains significant, but to a lesser degree in comparison with the vestibule and nasal valve regions, which is likely due to the increased flow area (decreased flow speed) and less severe streamline curvatures. Within the main passage, diffusion is enhanced in the middle and inferior meatus by the slow-moving flows (and the resulting prolonged particle residence times) as well as the large surface areas of these two fin-like projections available for particle contact. As a result, the deposition fraction of the DF-VC model is only 3.0 times that of the CS model for the middle meatus and 2.9 times larger for the lower passage.

Figure 11.14a shows the DF-VC simulation results of inspiratory deposition fractions in comparison to replica measurements as a function of a diffusion
Figure 11.14. Predicted deposition rates with the DF-VC model in comparison with existing in vitro experimental data for particles ranging from 1 to 1,000 nm and inhalation flow rates ranging from 4 to 45 L/min: (a) inspiratory, (b) expiratory. Units: $Q$ [L/min] and $D$ [cm$^2$/s].

As described earlier, the DF-VC approximation accounts for both particle inertia and diffusion, whereas the CS model only considers particle diffusion. As a result, the increased deposition of the DF-VC model over the CS approach can be attributed entirely to particle inertial effects. For ultrafine particles where inertial effects are negligible, the Sherwood number $Sh$ is nearly identical for the two models considered (Figure 11.15a). Deviation of $Sh$ between the DF-VC and CS models begins at $Re^{0.55}Sc^{0.60} = 1.5 \times 10^4$ (equivalently, $St_{k} = 1.0 \times 10^{-5}$) and becomes progressively significant with increasing values of $Re^{0.55}Sc^{0.60} (or St_{k})$. Compared with the inertial limit of $St_{k} = 5.0 \times 10^{-5}$ for TB airways [20], a smaller value in

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**Figure 11.14.** Predicted deposition rates with the DF-VC model in comparison with existing in vitro experimental data for particles ranging from 1 to 1,000 nm and inhalation flow rates ranging from 4 to 45 L/min: (a) inspiratory, (b) expiratory. Units: $Q$ [L/min] and $D$ [cm$^2$/s].

**Figure 11.15a.** Predicted deposition rates with the DF-VC model in comparison with existing in vitro experimental data for particles ranging from 1 to 1,000 nm and inhalation flow rates ranging from 4 to 45 L/min: (a) inspiratory, (b) expiratory. Units: $Q$ [L/min] and $D$ [cm$^2$/s].

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**Figure 11.15b.** Predicted deposition rates with the DF-VC model in comparison with existing in vitro experimental data for particles ranging from 1 to 1,000 nm and inhalation flow rates ranging from 4 to 45 L/min: (a) inspiratory, (b) expiratory. Units: $Q$ [L/min] and $D$ [cm$^2$/s].

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**Figure 11.16.** Predicted deposition rates with the DF-VC model in comparison with existing in vitro experimental data for particles ranging from 1 to 1,000 nm and inhalation flow rates ranging from 4 to 45 L/min: (a) inspiratory, (b) expiratory. Units: $Q$ [L/min] and $D$ [cm$^2$/s].

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**Figure 11.17.** Predicted deposition rates with the DF-VC model in comparison with existing in vitro experimental data for particles ranging from 1 to 1,000 nm and inhalation flow rates ranging from 4 to 45 L/min: (a) inspiratory, (b) expiratory. Units: $Q$ [L/min] and $D$ [cm$^2$/s].
The nasal cavity indicates an earlier onset of particle inertial effects, which may be due to the high complexity of this geometry.

While the nasal deposition can be reasonably predicted by existent empirical correlations in the literature, these expressions are typically limited to ultrafine or coarse particles where either diffusion or inertial impaction are the predominate mechanisms for particle loss. Therefore, a correlation that is valid for both diffusional and inertial deposition regimes is of value to inhalation toxicologists and is sought in this study based on numerical experiments. Figure 11.15 shows the development of a mass transfer correlation in the nasal cavity in terms of the non-dimensional Sherwood number. The dependence of mass transfer on convective diffusion is plotted in Figure 11.15a with a best-fit correlation for the diffusion zone given by

$$Sh = (Re^{0.55} Sc^{0.60})^{0.553} = Re^{0.30} Sc^{0.33} \quad (St_k \leq 1.0 \times 10^{-5})$$  \hspace{1cm} (19)$$

The convective–diffusion coefficient \((Re^{0.55} Sc^{0.60})\) adopted here was suggested by Cheng et al. [68] for in vivo nasal deposition data. For fine respiratory particles that are influenced by diffusion and impaction deposition mechanisms, the deviation from the above equation \((\Delta Sh, \text{see Figure 11.15a})\) due to particle inertia can be correlated as a function of \(St_k\) using (Figure 11.15b)

$$\Delta Sh = 4.7 \times 10^6 \ St_k^{1.1}$$  \hspace{1cm} (20)$$

Figure 11.15. Development of a Sherwood number Sh correlation in the nasal airway that accounts for both diffusional and inertial deposition mechanisms for submicrometer aerosols: (a) correlation for ultrafine particles where diffusion dominates deposition and (b) correlation for enhanced mass transport due to particle inertia, \(\Delta Sh\), as a function of Stokes number, \(St_k\).
Based on the assumption of weak coupling between the inertial and diffusive deposition mechanisms, the overall correlation that is valid for all submicrometer particle sizes can be obtained by adding equations (19) and (20) as:

\[ Sh = \text{Re}^{0.30} \text{Sc}^{0.33} + 4.7 \times 10^6 St_{k}^{1.1} \quad (d_p = 1 - 1,000 \text{ nm}) \] (21)

Alternatively, the above correlation can be expressed in terms of total nasal deposition fraction,

\[ Df = 1 - \exp \left[ -\left( \frac{A_s}{A_c} \right) \left( \text{Re}^{-0.70} \text{Sc}^{-0.67} + 4.7 \times 10^6 \frac{St_{k}^{1.1}}{\text{Re Sc}} \right) \right] \] (22)

where \( A_s \) is the total surface area and \( A_c \) the mean cross-sectional area of the nasal passage. The above equation is valid for particle size ranging from 1 to 1,000 nm.

### 11.7 Discussion

Numerical simulations of fine respiratory aerosols are challenging due to low deposition efficiencies and the action of concurrent inertial and diffusive deposition mechanisms. The CS Eulerian model that is typically applied for ultrafine aerosols is highly efficient and shows reasonable agreement with analytic solutions for ultrafine diffusive deposition in a tubular geometry [17,20,69]. However, the typical CS Eulerian model neglects the effects of finite particle inertia [20,32] and cannot be used to predict fine particles in the range of 100 to 1,000 nm. As presented in this chapter, finite particle inertia may significantly affect the total deposition of submicrometer aerosols as small as 70 nm and the local deposition of particles as small as 40 nm [25,40,42]. Based on the available two-phase flow literature, the standard DF model should adequately model the deposition of dilute fine respiratory aerosols based on diffusional and inertial transport mechanisms [32,33]. However, results presented by Longest and Oldham [25] and summarized above indicated a significant overprediction of respiratory aerosol deposition with the use of the standard DF formulation. This overestimation was due to significant changes in particle slip velocity between the near-wall control volume center location and conditions at particle-to-wall contact. To improve the simulations of submicrometer aerosols in the respiratory tract, a hybrid DF-VC model was developed and tested both experimentally and numerically [25,40,42]. In comparison with the CS model, deposition results of the DF-VC approach persistently agreed better with experimental findings on a total and subbranch basis, which indicated that the DF-VC model effectively captured the influence of finite particle inertia. Results of this study indicate that a DF particle transport model with near-wall velocity corrections can provide an effective approach for simulating the transport and deposition of submicrometer respiratory aerosols in complex human respiratory airways.

While the DF-VC model has been shown to be effective for submicrometer respiratory aerosols, it does have several limitations. The current DF-VC model was
developed mainly for submicrometer aerosols based on the use of the pressure gradient term in equation (11b). This model can also be extended to larger particle sizes if equation (11a) is used to compute particle slip. Another limitation of the general DF approach is the assumption of a dilute aerosol in which the momentum of the discrete phase does not influence the flow field. As a result, low loadings of particle concentration are required, which is generally the case for respiratory aerosols. Finally, the current model was developed for monodisperse aerosol distributions.

The results of the studies summarized in this chapter should not be interpreted to imply that the continuous field DF-VC model is superior to Lagrangian particle tracking for simulating aerosol transport in all situations. A primary advantage of Lagrangian particle tracking is the direct treatment of particles as individual or potentially interacting discrete elements, in contrast with the approximation of a continuous aerosol field. Treating particles as discrete elements allows for the direct evaluation of individual force terms that represent a number of physical phenomena such as lift, near-wall lubrication, and particle-to-particle interactions [29]. Furthermore, Lagrangian particle tracking can be directly applied to non-spherical shapes, like rotating fibers, and polydisperse aerosols. In contrast to the Lagrangian approach, the DF-VC model approximates finite particles as a continuous species. As a result, transport and deposition are evaluated from the solution of a convection–diffusion equation, which may introduce numerical dissipation errors into the solution. Furthermore, it does not appear that the DF-VC model can effectively account for particle-to-particle interactions or the motion and interception of complex shapes, like rotating fibers. A primary advantage of the DF-VC model is high efficiency, where successive additions of discrete particles are not required to establish converged local deposition characteristics. As a result of these observations, it is clear that both the continuous field DF-VC model and Lagrangian particle tracking have inherent strengths and weaknesses. Further testing and evaluation is required to extend the flexibility of the DF-VC model and to overcome some current limitations, such as monodisperse aerosols. It is likely that selection of Eulerian versus Lagrangian models for submicrometer aerosol transport will remain dependent on the particular problem of interest in conjunction with the advantages and disadvantages of each method. However, results of this study indicate that the DF-VC model does provide an effective approach that can simulate the concurrent action of diffusion and inertia in a complex transient and laminar-to-turbulent flow field.

In conclusion, a continuous-phase DF particle transport model with a near-wall velocity correction provided an effective solution for the deposition of submicrometer aerosols under transient and laminar-to-turbulent flow conditions. Comparisons with a standard CS model indicated that the DF-VC approach was incorporating the effects of finite particle inertia in determining total and local deposition characteristics for the complex TB and nasal geometries that were considered. Comparisons of steady and transient conditions indicated that cyclical flow decreased the total deposition of submicrometer particles but significantly increased relative particle localization, as indicated with the DEF parameter. Future studies are necessary to address wall surface roughness and compliance, mucus clearance, and real-life...
breathing waveforms before the current DF model can be directly applied to make dose–response and health effects predictions.

References

Computational Fluid Dynamics and Heat Transfer


