ABSTRACT
The hazard caused by inhaled particles depends on the site at which they deposit within the respiratory system. Knowledge of respiratory aerosol deposition rates and locations is necessary to (1) evaluate potential health effects and establish critical exposure limits and (2) design effective inhaled medications that target specific lung regions. Particles smaller than 10 µm in diameter can be breathed into lungs and are known as inhalable particles, while most of larger particles settle in mouth and nose. Inhalable particles settle in different regions of the lungs and the settling regions depends on the particle size. The motion of a particle is mainly affected by the inertia of the particle and by the particle’s aerodynamic drag. The most important dimensionless parameters in the prediction of particle motion are the flow Reynolds number and the Stoke number, which combines the effects of particle diameter, particle density, shape factor and slip factor.

The purpose of this study is to investigate the airflows in human respiratory airways. The influence of particle size on transport and deposition patterns in the 3-D lung model of the human airways is the primary concern of this research. The lung model developed for this research extends from the trachea to the segmental bronchi and it is based on Weibel’s model. The velocity field of air is studied and particle transport and deposition are compared for particles in the diameter range of 1 µm -100 µm (G0 to G2) and 0.1 µm - 10 µm (G3 to G5) at airflow rates of 6.0, 16.7, and 30.0 L/min, which represent breathing at rest, light activity, and heavy activity, respectively.

The investigation is carried out by computational fluid dynamics (CFD) using the software Fluent 6.2. Three-dimensional, steady, incompressible, laminar flow is simulated to obtain the flow field. The discrete phase model (DPM) is then employed to predict the particle trajectories and the deposition efficiency by considering drag and gravity forces.

In the present study, the Reynolds number in the range of 200 – 2000 and the Stoke number in the range of 10^-5 – 0.12 are investigated. For particle size over 10 µm, deposition mainly occurs by inertial impaction, where deposition generally increases with increases in particle size and flow rate. Most of the larger micron sized particles are captured at the bifurcations, while submicron sized particles flow with the fluid into the lung lower airways. The trajectories of submicron sized particles are strongly influenced by the secondary flow in daughter branches. The present results of particle deposition efficiency in the human upper airways compared well with data in the literature.

1. INTRODUCTION
The human airways are a complicated series of bifurcating tubes, from the trachea; the network splits into two main bronchi and continues to bifurcate throughout the conducting and pulmonary regions. The hazard caused by inhaled particles depends on the site at which they deposit within the respiratory system. Thus, it is necessary to understand how particles or aerosols behave and deposit in the lungs. In addition, the deposition efficiency of delivering drug aerosols is important for the drug industry to effectively design inhaled drug aerosol systems. The deposition of particles and aerosols to surfaces occurs in three major processes: direct gravitational settling to the surface, inertial impaction of particles on the surface, and Brownian diffusion of particles through the boundary layers of various surfaces. The subject of aerosol technology has been reviewed comprehensively by Hinds (1999) and Heinsohn and Cimbala (2003). Maynard and Kuempel (2005) have reviewed recent developments in airborne nanoparticles.

It is known that gravitational settling dominates for large particles (> 100 µm), inertial impaction dominates in middle size ranged particles around 10 µm, and Brownian diffusion dominates for very small particles (< 0.1 µm). Figure 1 shows particle diameters from natural processes (1 - 100 µm) such as pollen, mold, fungi, mist, fog, manmade pollution (0.01 - 1 µm) such as fume, oil smoke, tobacco smoke, aerosols used in drug delivery (1 - 6 µm), bacteria (0.2 - 20 µm) and virus (< 0.1 µm). Of particular interest in occupational health and
indoor air quality are PM 2.5 and PM 10, corresponding to particulate matters below 2.5 µm and 10 µm, respectively.

In the upper airways, deposition occurs mainly by inertial impaction. Thus, deposition fraction generally increases with increasing particle size and flow rate. Most particles over 10 µm are deposited in the nose, mouth, throat and larynx, while most of the larger micron sized particles are captured at the first bifurcation, while smaller micron sized particles flow with the fluid into the lungs upper airways (bronchi) and lower airways (bronchioles). Submicron sized particles penetrate deeply into the alveolar region and enter the blood stream through the alveolar wall and pulmonary capillary network.

Comer et al. (2001a, 2001b) analyzed flow structures and particle deposition patterns in double-bifurcation airway models using the CFX code. Zhang et al. (2002) validated the CFD model in terms of particle deposition efficiency in double bifurcation model under cyclic and steady inhalation conditions by comparing their results with data in the literature (Kim and Fisher, 1999). Calay et al. (2002) studied the unsteady respiratory airflow dynamics including secondary motions in the daughter airways and flow separations close to the carinal ridge. The deposition behavior of nanoparticles was reviewed by Maynard and Kuempel (2005), who found a minimum deposition efficiency for particles around 0.3 µm. They concluded that the deposition mechanism for particles below 0.3 µm is dominated by the Brownian motion. Wang and Lai (2006) developed a drift model to predict particle deposition fraction for particle size in the range from 1 nm to 10 µm; they determined minimum deposition efficiency for particle size around 0.4 µm as a result of weak Brownian motion combined with weak gravity force and weak inertia.

In this research the particle transport behavior and deposition patterns are investigated in a rigid, model of the human airways, extending from generations G0 to G5 (Fig. 2 and Table 1) based on the Weibel model (1963). The commercial Computational Fluid Dynamics (CFD) software package FLUENT is used for analysis of 3-D, steady, incompressible, laminar airflow. Both spherical (such as drug aerosols) and non-spherical particles (such as anthrax spores) with aerodynamic diameters in the range of 0.1 - 10 µm (inhaling particles) at inspiratory flow rates of 6, 17, and 30 L/min (representing sedentary, light activity, and heavy activity situations) are considered. Aerosol deposition studies have shown that deposition patterns of inhaled aerosols within airway bifurcations are inhomogeneous.

We will first validate our model considering larger particle deposition (1 - 100 µm) from generations G0 to G2 including trachea and bronchi. We will then study the detailed flow pattern including the secondary flow, particle trajectory and deposition efficiency for particle size from 0.1 to 10 µm in bronchioles G3 to G5.

**Figure 1.** Particle size and distribution in atmospherical air

**Figure 2.** 3D lung model (G0-G2 or G3-G5)

**Table 1.** Lung model geometry

<table>
<thead>
<tr>
<th>Model</th>
<th>Diameter(D)</th>
<th>Length(L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>G0</td>
<td>1.64</td>
<td>9.05</td>
</tr>
<tr>
<td>G1</td>
<td>1.19</td>
<td>3.76</td>
</tr>
<tr>
<td>G2</td>
<td>0.84</td>
<td>3.0</td>
</tr>
<tr>
<td>G3</td>
<td>0.56</td>
<td>0.76</td>
</tr>
<tr>
<td>G4</td>
<td>0.45</td>
<td>1.27</td>
</tr>
<tr>
<td>G5</td>
<td>0.35</td>
<td>1.07</td>
</tr>
</tbody>
</table>

**Bifurcation half-angle(θ)** | 30°

### 2. THEORY

#### 2.1 Gas transport equation

For steady, incompressible and laminar flow with constant properties, the gas transport is governed by the Navier-Stokes equations given as (Munson et al., 2006):

(continuity) \[ \mathbf{V} \cdot \nabla \bar{V} = 0, \]  \hspace{1cm} (1)

(momentum) \[ \left( \mathbf{V} \cdot \nabla \right) \bar{V} = -\frac{1}{\rho} \nabla P + \nu \nabla^2 \bar{V} + \ddot{g} \]  \hspace{1cm} (2)
where $\vec{v}$ is the velocity vector, $P$ is the pressure, $\rho$ is the fluid density, $\nu$ the fluid kinematic viscosity, and $\bar{g}$ is the gravitational acceleration.

### 2.2 Model geometry and flow properties

In order to investigate the particle deposition in human upper airways, the symmetric planar double bifurcation model, representing human respiratory airways, has been considered as shown in Figure 2. This model has been designed following the description of Weibel (1963) concerning lung geometry as outlined in Table 1. The numbering of these generations is based on Weibel’s convention including trachea, bronchus, and bronchiale (G0-G5). The air properties are based on standard atmosphere.

The flow Reynolds number, representing the ratio of inertial force to viscous force of the air flow, is defined as,

$$Re = \frac{\rho V_o D_0}{\mu}$$

where $\rho$ is the air density, $V_o$ is the average air velocity at the inlet, $D_0$ is the inside diameter of the first airway considered (G0 or G3), and $\mu$ is the air viscosity. The particle Reynolds number, representing the ratio of inertial force to viscous force of the particle, is defined as,

$$Re_p = \frac{\rho V_o d_p}{\mu}$$

where $d_p$ is the particle diameter and other variables are the same as those in Eq. (1). Particles greater than 10 µm are either settled to the ground or filtered out by the head airways including nose hair or mucus in the mouth, pharynx, and larynx, and thus do not enter the upper airways in the lungs. The inlet air flow rate and velocity & flow Reynolds numbers are listed in Table 2. The particle Reynolds number ranges from 0.003 to 1.31 in the present study.

<table>
<thead>
<tr>
<th>Physical state</th>
<th>Inlet air flow rate</th>
<th>Inlet air velocity (G0)</th>
<th>Re (G0)</th>
<th>Re (G3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sedentary</td>
<td>6 L/min</td>
<td>0.470 m/s</td>
<td>528</td>
<td>181</td>
</tr>
<tr>
<td>Light activity</td>
<td>17 L/min</td>
<td>1.317 m/s</td>
<td>1479</td>
<td>507</td>
</tr>
<tr>
<td>Heavy activity</td>
<td>30 L/min</td>
<td>2.370 m/s</td>
<td>2662</td>
<td>914</td>
</tr>
</tbody>
</table>

### 2.3 Particle Tracking and Stokes’s Law

Applying Newton’s 2nd law to each individual particle and assuming no interaction between particles and between particles and walls yield,

$$\Sigma F_p = m \frac{D\vec{v}}{Dt} = \vec{F}_L + \vec{F}_D + \vec{F}_G + \vec{F}_b$$

where $F_L$ is the lift force, $F_D$ is the drag force, and $F_G$ is the gravity force, and $F_b$ is the buoyancy force. In the case of spherical particles without spinning, the average lift force is zero. In the case of cylindrical particles, both $F_L$ and $F_D$ depend the shape and orientation of the particle relative to the air flow. It was found that a rod (such as anthrax) in its vertical position is unstable because the center of aerodynamic pressure is ahead of its center of gravity in the downward motion. As a result, the rod will rotate until it falls into a stable, horizontal position without considering the random Brownian motion. The buoyancy force is negligible in the present study because of $\rho << \rho_p$. Therefore, both $F_L$ and $F_b$ are neglected in the present numerical analysis.

Stokes’s law assumes that the fluid is incompressible, there are no walls or other particles nearby, the motion of the particles is constant, the particle is a rigid sphere, and the fluid velocity at the particle’s surfaces is zero. The net force acting on the particle is obtained by integrating the normal and tangential forces over the surface of the particle. The total resisting force on a spherical particle moving with a velocity $V$ through a fluid is:

$$F_D = 3\pi \mu V d_p$$

### Terminal settling velocity

When a small particle is released in air, it quickly reaches its terminal settling velocity, a condition of constant velocity wherein the drag force of the air on the particle, $F_D$, is exactly equal and opposite to the force of gravity, $F_G$. Under this condition, Eq. (5) is reduced to

$$F_D = F_G = mg$$

where $g$ is the acceleration of gravity. Combining Eqs. (6) and (7) yields the terminal settling velocity $V_T$:

$$V_T = \frac{\rho_p d^2 g}{18 \mu}$$

### Slip correction factor

An important assumption of Stokes’s law is that the relative velocity of the gas right at the surface of the sphere is zero. This non-slip boundary condition is not valid for small particles ($d_p < 1\mu m$) whose size approaches the mean free path of the gas. To take into account the slip flow on small particles, the Cunningham correction factor $C_c$ based on Brownian diffusion in the viscous sublayer [Ounis et al., 1991] can be used to determine the drag force. Since $C_c$ is always greater than one, the Stokes drag force is reduced as [Faghri and Sunden, 2004]:

$$F_D = F_D^{C_c}$$

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\[
F_D = \frac{3\pi\mu V d_p}{C_c} \quad (9)
\]

\[
C_c = 1 + 2 \cdot Kn[1.257 + 0.4 \exp\left(\frac{0.55}{Kn}\right)] \quad (10)
\]

Three regimes can be classified according to the value of the Knudsen number as follows:

- \( Kn < 0.1 \) continues regime
- \( 0.1 < Kn < 10 \) transitional flow regime
- \( Kn > 10 \) free molecular flow regime (not considered in this study)

The Knudsen number \( (Kn) \) is used to distinguish the two regimes and is defined as:

\[
Kn = \frac{\lambda}{d_p} \quad (11)
\]

The average distance traveled by air molecules between collisions with each other is called mean free path \( (\lambda) \). Mean free path can be expressed as [Faghri and Sunden, 2004]

\[
\lambda = \frac{\mu}{0.499 \sqrt[8]{\pi / 8}} \quad (12)
\]

For air in the standard atmosphere, the mean free path is 66 nm. The slip-corrected form of the terminal settling velocity becomes

\[
V_{ts} = \frac{\rho_o d_v^2 g C_c}{18\mu} \quad \text{for } Re < 1 \quad (13)
\]

The Cunningham correction factor as a function of particle diameter is shown in Fig. 3. For particles above 3 µm, \( C_c \approx 1 \) and for particles from 0.1 to 3 µm, \( C_c \) varies from 3.0 to 1.1.

### 2.4 Equivalent volume diameter and dynamic shape factor

A correction factor called the dynamic shape factor is applied to Stokes’s law to account for the effect of shape on particle motion. The dynamic shape factor is defined as the ratio of the actual resistance force of the nonspherical particle to the resistance force of a sphere having the same volume and velocity as the nonspherical particle.

\[
\chi = \frac{F_D}{3\pi\mu V d_v} \quad (14)
\]

Where \( d_v \), called the equivalent volume diameter, is the diameter of a sphere having the same volume as that of an irregular particle.

### 2.5 Aerodynamic diameter

The Aerodynamic diameter is defined as the diameter of the spherical particle with a density of 1000 kg/m³ (the density of a water droplet) that has the same settling velocity as the particle. Equation (13) can be written in terms of this diameter, neglecting slip correction, as

\[
V_{ts} = \frac{\rho_o d_v^2 g}{18\mu\chi} \quad (16)
\]

where \( \rho_o \) is the standard particle density, 1000 kg/m³. The aerodynamic diameter can be thought of as the diameter of a water droplet having the same aerodynamic properties as the particle. For particles greater than 100 µm, the settling velocity is over 0.25 m/s in standard air, which is too large to be airborne. Thus, they are considered not inhalable.

### 2.6 Stokes number

Very small particles with negligible inertia will follow the gas streamlines perfectly around an obstacle while large and heavy particles with large inertia will tend to continue in a
straight line. When a particle follows a curved path it is said to have curvilinear motion. Curvilinear motion is characterized by a dimensionless number called the Stokes number (St). It is the ratio of the stopping distance of a particle to a characteristic dimension of the obstacle. For flow in the upper airways, the Stokes number is defined as,

\[ St = \frac{rV}{D_o}, \quad \text{for} \ Re < 1 \]  

(17)

where \( V_o \) is the inlet velocity of air, \( D_o \) is the inlet airway diameter, and \( r \) is the relaxation time of the particle (Heinsoln and Cimbala, 2003; Hinds, 1999),

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

(18)

Clearly, \( V_{ts} = \tau g \) and the aerodynamic diameter is,

\[ d_a = d_p \left( \frac{\rho_p}{\rho_e} \right)^{1/2} \]  

(19)

The relaxation time \( (\tau) \) characterizes the time for a particle to adjust or relax its velocity to a new condition under either a gravitational force or a viscous force. The Stoke number also represents the ratio of the particle relaxation time to the radial traversal time across the airway diameter, as well as the ratio of particle inertial force \( (F_I) \) to drag force \( (F_D) \) on the particle.

When \( St >> 1 \) \( (F_I >> F_D) \), particles continue moving in a straight line when the gas turns; when \( St << 1 \) \( (F_I << F_D) \), particles follow the gas streamlines. As the Stoke number approaches zero, particles track the streamlines perfectly. The Stoke number as a function of particle diameter and air inlet velocity is shown in Fig. 4.

### 2.7 Dimensional Analysis

By neglecting the buoyancy force and the lift force (see Section 2.3), the force acting on the particle by the fluid flow is mainly balanced by the inertial, viscous and gravitational forces,

\[ \vec{F} = f(\vec{F}_I, \vec{F}_D, \vec{F}_G) \]  

(20)

Clearly, we have \( F_I \sim \rho V^2 d_p^2 \), \( F_D \sim \mu V d_p \) and \( F_G \sim \rho g d_p^3 \). Therefore, the gravitational forces dominate for large particles, the viscous force dominate for small particles, and the inertial force plays an important role for particles in the range of 0.1 – 10 \( \mu \)m in the present study.

While the Reynolds number in Eq. (3) characterizes the flow field, the Stoke number is the most important dimensionless parameter in particle dynamics because it combines the effects of the particle diameter, particle density and shape factor, \( \chi \).

### 3. NUMERICAL METHOD

#### 3.1 CFD modeling

The numerical solution of fluid flow equations (Eqs.(1) and (2)) were carried out employing a user-enhanced program, FLUENT (version 6.2), which is developed based on a finite volume technique and pressure-based segregated solution algorithms. A companion package to FLUENT, called GAMBIT provides geometry generation, geometry import, and mesh generation capabilities. Velocity fields were converged on each of the subunit lung geometries using the finite volume method within FLUENT.
3.2 Building the model

The computational mesh was generated by GAMBIT. The geometry of the model in section 2.2 was created and meshed with tetrahedral cells for the better flexibility in adapting to curved surfaces. In the radial direction, a much finer mesh was implemented around the surfaces of wall to improve solution by refining the grid to better resolve the flow details. Adapting the grid was performed using the tutorial supplied by Fluent. The grid adaptation used for this work was based on velocity gradient so that finer grids can be generated in locations where there is a large change in velocity, such as along the walls.

3.3 Boundary conditions

The inlet boundary condition at G0 or G3 is assumed to follow the fully-developed, laminar velocity profile. The choice of boundary conditions for the outlet is important for these simulations and two possibilities exist: (1) pressure conditions, where the pressure at each outlet is specified, or (2) outflow conditions where the fraction of the total volumetric flow at the inlet and at an outlet is specified. Based on their observations, Nowak et al. (2003) concluded that the constant pressure outlet boundary conditions would yield an insignificant deviation from outflow approximation in particle tracking calculations. Therefore, it was decided to use constant pressure outlet boundary conditions in the rest of this work and it was assumed that the pressure is zero at outlet. A particle is trapped on a wall surface when it hit the wall and particle tracking is terminated.

3.4 Grid adaptation

To improve the accuracy near regions of large velocity gradients, the grid adaptation was used by refining the mesh near wall surfaces. Figure 5 shows the grid adaptation at the inlet and the outlet of G2. Similar non-uniform grids are used in all branches.

![Figure 5. Grid adaptation at inlet(G2)](image)

3.5 Particle Trajectory Calculation

FLUENT predicts the trajectory of discrete phase particles by integrating the force balance on each particle, which is written in a Lagrangian reference frame. The discrete phase modeling with FLUENT requires the assumption that there is no particle-particle interactions and the particles do not break up. Also the effects of the particle volume fraction on the gas phase should be less than 10-12%. The force balance equates the particle inertia with the drag and gravity forces acting on the particle, and can be written as

\[
\frac{d\vec{V}_p}{dt} = f_D(\vec{V} - \vec{V}_p) + \frac{g_z(\rho_p - \rho)}{\rho_p} \tag{24}
\]

where \( f_D(\vec{V} - \vec{V}_p) \) is the drag force per unit particle mass (acceleration due to drag) and

\[
f_D = \frac{18\mu C_D Re_r}{\rho_p d_p^2} \frac{Re_r}{24} \tag{25}
\]

Here, \( V \) is the fluid phase velocity, \( V_p \) is the particle velocity, \( \mu \) is the dynamic viscosity of the fluid, \( \rho \) is the fluid density, \( \rho_p \) is the density of the particle, and \( d_p \) is the particle diameter. \( Re_r \) is the relative Reynolds number, which is defined as

\[
Re_r = \frac{\rho d_p |V_p - V|}{\mu} \tag{26}
\]

The drag coefficient, \( C_D \) is calculated using the following expression:

\[
C_D = a_i + \frac{a_s}{Re_r} + \frac{a_2}{Re_r^2} \tag{27}
\]

where \( a_i \) are constants that apply to smooth spherical particles over several ranges of \( \text{Re} \) given by Morsi and Alexander (1972). For sub-micron particles (< 0.1 µm), the Cunningham correction factor from Eq. (10) can be used,

\[
f_D = \frac{18\mu}{d_p^2 \rho_p C_c} \tag{28}
\]

In FLUENT, the default gravitational acceleration is zero. Thus the magnitude and direction of the gravity vector must be defined. This differential force balance was integrated over time to yield the displacement as a function of time. Particles of specific sizes were introduced in a uniform distribution at the inlet face of the computational domain, and tracked through the geometry till they met one of three fates: (1) trapping on a surface by collision, (2) escape from the domain through one of the outlet faces, or (3) continued suspension in the flow. The fate of the particles were then recorded and summarized as a particle history file. Both the flow field and particle trajectory calculations were performed primarily on a 3.39 GHz Pentium® D processor and took a few minutes per calculation.
4. RESULTS

4.1 Model validation for particle diameter (G0-G2, 1-100µm)

After the flow field is determined by solving Eqs. (1) and (2), the particle trajectories of different particle sizes released at the same point are then calculated. As shown in Fig. 6, larger particles (>50 µm) are captured at the carina region, in which the inertial impaction dominates. Smaller particles (<20 µm) with lower Stoke number reach further down to lower airways because the drag force \( F_D \) becomes increasingly important as compared with the inertial force \( F_I \). As shown in Fig. 7, particle deposition fraction increases with increasing particle diameter in the particle diameters in the range of 1-100µm (G0-G2). The particle deposition fraction (DF) increases drastically in the range of 10 – 100µm. Note that particles over 10 µm are not inhalable because they are captured in the head airways as a result of high terminal settling velocity. The particles greater than 10 µm are removed by settling and by impaction on nasal hairs and at bends in the airflow path. Particle deposition fraction also increases as air flow rate increases. The present study agrees with the prediction by Hogberg (2006) with a flow rate of 30 L/min.

![Figure 6. Particle trajectories (G0-G2, 1-100µm)](image)

![Figure 7. Deposition fraction vs. particle without the effect of inhalability diameter (G0-G2, 1-100µm)](image)

4.2 Velocity field (G3-G5)

Figure 8 shows the velocity field by assuming a fully-developed, parabolic inlet velocity with an average velocity of 2.37 m/s. The velocity contours in Fig. 8(a) shows the maximum velocities decrease from G3 to G5. The velocity profiles in Fig. 8(b) are skewed in the first daughter branches and higher velocities occur near the carina region (bifurcation) and along the inner walls. Consequently, a higher air velocity presents inside second daughter branches. The velocity profiles in Fig. 8(b) are in good agreement with those in Comer et al. (2001a) and Calay et al. (2002).

![Figure 8. Velocity field for a fully developed inlet velocity condition: (a) velocity contours and (b) velocity vectors.](image)

4.3 Secondary flow (G3-G5)

Figure 9 shows the airway model with cross sections for detailed flow field and particle trajectory analysis.

![Figure 9. Airway model with locations of velocity cross-sections](image)

Secondary flow vectors at the cross-sectional plane B-B’ and D-D’ are depicted in Figure 10. The secondary flow vectors on D-D’ plane are scaled up to show their directions. In fact the magnitude of the vectors on B-B’ (Fig. 10(a)) is greater than D-D’ (Fig. 10(b)) and it results in stronger secondary flow effect in B-B’ region (see Fig.11). After the air flow passes the first bifurcation A-A’, the vortices are formed due to the pressure gradient in the normal direction \( (P_B - P_B' = 0.2 \text{ Pa} \) and \( P_D - P_D' = 0.1 \text{ Pa} \)) that drives the slower moving fluid from the outside wall towards the inside wall. Similar secondary flow patterns were illustrated by Zhang et al. (2002).
Figure 10. Velocity vectors for secondary flow in G4-G5 for $V_o = 0.47\text{m/s}$.

Figure 11 shows the comparison of axial and secondary flow velocity magnitude between two different air velocities at two planes (B-B' & D-D'). The stronger secondary flow appears at higher inlet air velocity ($V_o = 0.47\text{m/s}$) and upper daughter branches (B-B'). The secondary flow is less pronounced at D-D' than at B-B'.

Figure 11. Axial vs. Secondary velocity magnitude

4.4 Particle trajectories

FLUENT tracks each of the released particles and stops tracking as soon as the particle hits and sticks to the wall surface. Fig. 12(a) and (b) depict different trajectories of two particles ($d_p = 1$ and $10 \mu\text{m}$) which are released at the same location at the inlet (G3) with an inlet air velocity of $1.317\text{m/s}$. It is shown that the larger particle ($d_p=10 \mu\text{m}$) is deposited at the carina ridge while the smaller particle ($d_p=1 \mu\text{m}$) escape the airway model through the outlet (G5). The smaller particle can follow the streamlines and avoid hitting the wall surface until it flows out of the model. However the larger particle whose inertia exceeds a certain value is unable to follow the streamlines. It makes impact on the surface and is deposited.

Most particles (over 98%) smaller than $1 \mu\text{m}$ do not deposit but escape through the outlets (G5). Fig. 13(a) and (b) compare the trajectories of specifically chosen particles ($d_p=0.1 \mu\text{m}$), released at the same location at the inlet (G3) with two different air velocities ($V=0.47 \text{m/s}$ & $V=2.37 \text{m/s}$). The particle in Fig. 13(a) escapes the airway model at lower inlet air velocity while Particle (b) is deposited at second bifurcation region at higher inlet air velocity. The deposition of the particle in Fig. 13 (b) near the second bifurcation (G4-G5) may be attributed to the stronger secondary flow as shown in Fig. 11 (b).

Figure 12. Trajectories of particles with two different particle diameters ($V_o =1.317 \text{m/s}$)

Figure 13. Trajectories of a particle with two different inlet air velocities ($d_p=0.1 \mu\text{m}$)

Trajectories of selected particles (0.1 $\mu\text{m}$) are shown in Fig. 14(a). The different colors represent different particles released at different locations. Fig. 14(b) portrays the trajectory of a single particle (orange colored particle) which is strongly influenced by the secondary flow as shown by the spiral motion. This particle follows the vertical flow in G3 until near the first carina region (A-A’) and is pulled away from the inner wall to the outer wall in G4. Smaller particles ($d_p<10 \mu\text{m}$) with low inertia do not deposit at bifurcations, but a fraction of them could be deposited in bronchiole walls in G4 due to the secondary flows. Comer et al. (2001b) found that the secondary flow is stronger for higher Reynolds number cases and the smaller particles are strongly affected by the secondary flow.
4.5 Particle Deposition

The number of particles injected at inlet was 1415. The Deposition Fraction (DF) is defined as

\[
DF = \frac{\text{Number of Deposited Particle}}{\text{Number of Injected Particle}} \times 100
\]  

As shown in Fig. 15, the number of particles (d_p=3-10 µm) deposited during inhalation increases with increasing particle size because of inertial impaction. Increasing air flow rate generally increases the deposition fraction, which is consistent with the result from Hogberg (2006) and Zhang et al. (2005). Deposition fraction (DF) in the G3-G5 airways vs. inhalation flow and particle diameter (d_p=0.1-3 µm) is around 1-2% and almost constant. Because over 98% of the particles under 1 µm closely follow the flow field of the air, oil particles about 1 µm are often used as tracing particles in particle image velocimetry (Stanislas et al., 2000). Zhang et al. (2005) compared the micro- and nano-size particle depositions in a human upper airway model from G0 to G3; they also reported minimum deposition fraction (under 2%) for particle size from 0.1 to 1 µm.

Table 4 lists the aerodynamic diameter, particle relaxation time, terminal settling velocity, Stoke number, Knudsen number, and deposition fraction for spherical particles from 0.1 µm to 10 µm as well as Anthrax with a diameter of 1 µm and a length of 4 µm. For particles less than 3 µm, the ratios of V_{ts} to V_0 are very small (< 0.01), indicating a negligible gravity force as compared with the drag force (see Eq. (22)) so that the particle dynamics is dominated by the drag force. This results in a very low deposition fraction about 1-2%.

Table 4. Summary of particle dynamics for spherical and non-spherical particles (Anthrax in horizontal orientation)

<table>
<thead>
<tr>
<th>d_p(µm)</th>
<th>( \tau ) (s)</th>
<th>( V_0 ) (m/s)</th>
<th>St</th>
<th>Kn</th>
<th>DF(%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10µm</td>
<td>10</td>
<td>3.12 x 10^4</td>
<td>3.06 x 10^4</td>
<td>7.34 x 10^{-7}</td>
<td>0.0066</td>
</tr>
<tr>
<td>3 µm</td>
<td>3</td>
<td>2.91 x 10^5</td>
<td>2.86 x 10^4</td>
<td>6.85 x 10^{-3}</td>
<td>0.022</td>
</tr>
<tr>
<td>1x4µm  (Anthrax)</td>
<td>1.6</td>
<td>9.28 x 10^6</td>
<td>9.10 x 10^3</td>
<td>2.18 x 10^{-3}</td>
<td>0.066</td>
</tr>
<tr>
<td>0.3 µm</td>
<td>0.3</td>
<td>4.33 x 10^5</td>
<td>4.25 x 10^4</td>
<td>1.02 x 10^{-3}</td>
<td>0.220</td>
</tr>
<tr>
<td>0.1 µm</td>
<td>0.1</td>
<td>8.87 x 10^6</td>
<td>8.70 x 10^3</td>
<td>2.09 x 10^{-3}</td>
<td>0.660</td>
</tr>
</tbody>
</table>
5. CONCLUSIONS

In this present work, micron-sized particles are simulated for a human upper airway lung model, representing the Weibel model, under the laminar flow region. A numerical human lung model has been developed with realistic airflow using the CFD software, FLUENT. Simulation of particle transport and deposition in the model is demonstrated. From dimensional analysis, the deposition fraction is found to be a function of the flow Reynolds number and the Stoke number. In the present study, the Reynolds number in the range of 200 – 2000 and the Stoke number in the range of $10^{-5}$ – 0.12 are investigated.

Both spherical and cylindrical particles are investigated. Three different air flow rate during inspiration are considered. The particle deposition on the upper region (G0-G2) of airways generally increases with increase in particle size, which is to be expected. Larger particles above 10 µm with strong inertia are deposited to a great extent, and most of the particles are captured at the inner wall surface of first daughter branches. Micron sized particles in the diameter range 1-10 µm penetrate deep into lower airways. Submicron particles (< 1 µm) with low inertia are strongly affected by the secondary flow even under low flow rate conditions. The deposition fraction in G3 – G5 is found to be around 1-2%.

REFERENCES