CFPD Simulation of Radioactive Particle Deposition in Lungs

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ABSTRACT

In this study, we investigate local deposition of aerosol particles in bronchial system. Models are formed with the assumption of three-stage bifurcation of bronchia and the computational grid is constituted using GAMBIT software of computational fluid dynamics code FLUENT. Calculations are carried out for a variety of flow models available in FLUENT and for different particle intake flow rates and particle diameters. It is shown that $k$-$\omega$ and low Reynolds number $k$-$\varepsilon$ models of FLUENT such as AB, AKN and CHC produce results which are in perfect agreement among themselves and with the literature for particle deposition computations. It is also shown that standard $k$-$\varepsilon$ model is not suitable for analysing aerosols deposition in human respiratory system. Considering the fact that the dose distribution due to the deposited particles in lungs rather than its average value is more crucial, it is demonstrated in this work that computational fluid particle dynamics CFPD simulations are very convenient tools to estimate local depositions of radioactive aerosols. Based on the deposition models presented in the current study, local dose distribution in lungs due to radioactive aerosol particles intake could be determined as a further step.

1 INTRODUCTION

Simulation of human respiratory system is very difficult to determine local depositions. Therefore, such information has been inevitably tried to obtain from validated computational fluid-particle dynamics (CFPD) simulations which provide a non-invasive, accurate, and cost-effective means. Nevertheless, presently CFPD analyses are restricted to segments or regions of the respiratory system [1]. Hence, global lung deposition models [2-3], relying on experimental deposition correlations, algebraic and first order rate equations, or stochastic modelling approaches, are still valuable to readily obtain averaged particle deposition data. Since the dose distribution due to the deposited radioactive particles in lungs rather than its average value is more crucial local distributions of inhaled aerosols in the large central human airways are studied by using the FLUENT CFD code. These simulations highlight the effects of particle diameter, turbulent models, and flow rate on particle deposition patterns in lungs.
2 THEORY

2.1 Airway geometry

In general, the lungs consist of a series of bifurcating tubes, where each bifurcation leads to a new lung generation numbered 1-23. The first and still widely used mapping of the human lung was done by Weibel [4] in 1963, known as the symmetric planar Weibel A model. Improvements were published such as Finlay et al. [5] among others. Cytological studies of uranium miners show that the lung cancers have usually developed in the airway generations 3-5, where the primary deposition velocities are the highest. Thus, it is rather important to study the deposition of inhaled aerosol particles in this part of human airways in order to find relationship between the cellular dose and adverse health effects. In this work, the GAMBIT software is used for formation of 3D mesh structure of computational domain. In this work, the symmetric triple bifurcation model is used to simulate the airways through generations 3 to 6 as shown in Figure 1.

![Figure 1: Schematic of a symmetric triple bifurcation airway (generations G3-G6).](image)

The unstructured grid is employed. The near wall meshes are refined to have a $y+$ value around 1. This $y+$ value allows utilizing enhanced wall treatment for standard k-e turbulence model. The number of 3D cells employed in the present simulations is around 400,000. Further increase in the number of computational cells did not change calculated results significantly. The sizes used in this study regarding to each airway are the ones taken from improved mapping of the human lung of Finlay [5] as tabulated in Table 1.

<table>
<thead>
<tr>
<th>Generation</th>
<th>Finlay et al. model length (cm)</th>
<th>Finlay et al. model diameter (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>2.281</td>
<td>0.885</td>
</tr>
<tr>
<td>4</td>
<td>1.78</td>
<td>0.706</td>
</tr>
<tr>
<td>5</td>
<td>1.126</td>
<td>0.565</td>
</tr>
<tr>
<td>6</td>
<td>0.897</td>
<td>0.454</td>
</tr>
</tbody>
</table>
2.2 Governing Equations

2.2.1 Governing Equations for Air Flow

One of the objectives of this study is to investigate turbulent models effects on particle deposition. The conservation equations for mass, momentum and energy and turbulent models used in this study are outlined below.

2.2.1.1 Standard and Low Reynolds $k$-$\varepsilon$ Models

The continuity, Reynolds averaged Navier-Stokes equation and time-averaged energy equation are given as follows [6]:

$$\frac{\partial u_i}{\partial x_i} = 0, \quad (1)$$

$$\rho u_i \frac{\partial u_i}{\partial x_i} = - \frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_i} \left[ \mu \left( \frac{\partial u_i}{\partial x_i} + \frac{\partial u_j}{\partial x_j} \right) - \rho u_i u_j \right], \quad (2)$$

$$\rho c_p u_i \frac{\partial T}{\partial x_i} = \frac{\partial}{\partial x_i} \left[ k \frac{\partial T}{\partial x_i} - \rho u_i T \right], \quad (3)$$

where $u_i$ and $u_j$ are the velocity components in $x$ and $y$ directions, respectively, $\rho$ is the density, $P$ is the pressure, $\mu$ is dynamic viscosity, $c_p$ is the specific heat, $T$ is the temperature, $k$ is the thermal conductivity.

The Reynolds stress is related to the local velocity gradients by an eddy viscosity $\nu_t$ by using the Boussinesq approximation. The turbulence scalar quantities $k$ and $\varepsilon$ used to calculate $\nu_t$ are obtained from the following modelled transport equations:

$$\rho u_i \frac{\partial k}{\partial x_i} = \frac{\partial}{\partial x_i} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right] + \mu_t \left( \frac{\partial u_i}{\partial x_i} + \frac{\partial u_j}{\partial x_j} \right) \frac{\partial u_j}{\partial x_i} - \rho \nu_t \varepsilon, \quad (4)$$

$$\rho u_i \frac{\partial \varepsilon}{\partial x_i} = \frac{\partial}{\partial x_i} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_i} \right] + f_1 C_1 \mu_t \frac{\varepsilon}{k} \left( \frac{\partial u_i}{\partial x_i} + \frac{\partial u_j}{\partial x_j} \right) \frac{\partial u_j}{\partial x_i} - \rho f_2 C_2 \frac{\varepsilon^2}{k} + E, \quad (5)$$

$$\mu_t = \rho f_3 C_\mu \frac{k^2}{\varepsilon}, \quad (6)$$

$$\bar{\varepsilon} = \varepsilon + D, \quad (7)$$

$$Re_x = \frac{\rho k^2}{\mu \varepsilon}, \quad Re_y = \frac{\rho \sqrt{ky}}{\mu}, \quad Re_z = \frac{\rho (\mu \varepsilon / \rho)^{1/4} y}{\mu} \quad (8)$$

where $C_\mu, C_1, C_2, \sigma_k$ and $\sigma_\varepsilon$ are the same empirical turbulence model constants to those conveniently in the high Reynolds number $k$-$\varepsilon$ model. In the current study following values are used for the model constants: $C_\mu = 0.09, C_1 = 1.44, C_2 = 2.93, \sigma_k = 1.0$ and $\sigma_\varepsilon = 1.3$. The dumping functions $f_\mu, f_1$ and $f_2$, and $D$ and $E$ terms are used to make the low Reynolds number models valid in the near wall region. The detailed physical meaning of the dumping functions and the $D$ and $E$ terms is given in Ref. [7]. The dumping functions for the various low Reynolds number $k$-$\varepsilon$ models used in this work are summarized in Tables 2.
Table 2: Summary of dumping functions appearing in governing equations

<table>
<thead>
<tr>
<th>Model</th>
<th>$f_\mu$</th>
<th>$f_1$</th>
<th>$f_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard</td>
<td>1.0</td>
<td>1.0</td>
<td>$\left[ 1 - \frac{2}{9} \exp(-\text{Re}_T^2) / 36 \right]^2$</td>
</tr>
<tr>
<td>$k-\varepsilon$</td>
<td>tanh $\left( 0.008 \text{Re}_T \right) \left( 1 + 4 \text{Re}_T^{-3/4} \right)$</td>
<td>1.0</td>
<td>$\left[ 1 - \frac{\text{Re}_T}{12} \right]$</td>
</tr>
<tr>
<td>AB</td>
<td>$\left{ 1 + 5.0 / \text{Re}_T^{3/4} \exp\left[ - \left( \text{Re}_T / 200 \right)^2 \right] \right}$</td>
<td>1.0</td>
<td>$\left[ 1 - 0.3 \exp\left[ -\left( \text{Re}_T / 6.5 \right)^2 \right] \right]^2$</td>
</tr>
<tr>
<td>AKN</td>
<td>$\left[ 1 - \exp(-\text{Re}_T / 14) \right]^2$</td>
<td>1.0</td>
<td>$\left[ 1 - \left( \text{Re}_T / 3.1 \right)^2 \right]$</td>
</tr>
<tr>
<td>CHC</td>
<td>$\left[ 1 - \exp(-0.0215 \text{Re}_T) \right]^2 \left( 1 + 31.66 / \text{Re}_T^{5/4} \right)$</td>
<td>1.0</td>
<td>$\left[ 1 - 0.01 \exp(-\text{Re}_T^2) \right]$</td>
</tr>
</tbody>
</table>

Low Reynolds number turbulent models such as AB, AKN and CHC models tabulated in Table 2 are not associated with the wall laws but make it to predict effectively the dynamic, thermal, and turbulent behaviour of pipe flows.

### 2.2.1.2 Standard $k$-$\omega$ Model

The standard $k$-$\omega$ model is an empirical model based on modelled transport equations for the turbulence kinetic energy ($k$) and the specific dissipation rate ($\omega$) which can also be thought as the ratio of $\varepsilon$ to $k$.

The transport equations for the standard $k$-$\omega$ model are:

\[
\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial z_i} (\rho k U_i) = \frac{\partial}{\partial z_j} (\Gamma_k \frac{\partial k}{\partial z_j}) + G_k - Y_k + S_k, \tag{9}
\]

\[
\frac{\partial}{\partial t} (\rho \omega) + \frac{\partial}{\partial z_i} (\rho \omega U_i) = \frac{\partial}{\partial z_j} (\Gamma_\omega \frac{\partial \omega}{\partial z_j}) + G_\omega - Y_\omega + S_\omega.
\]

In these equations, $G_k$ represents the generation of turbulence kinetic energy due to mean velocity gradients. $G_\omega$ represents the generation of $\omega$. $\Gamma_k$ and $\Gamma_\omega$ represent the effective diffusivity of $k$ and $\omega$, respectively. $Y_k$ and $Y_\omega$ represent the dissipation of $k$ and $\omega$ due to turbulence. $S_k$ and $S_\omega$ are user-defined source terms.

### 2.2.2 Governing Equations for Particle Motion

Motion of radioactive aerosol particles suspended in the inhaled air is analyzed by using discrete phase model of FLUENT. The particle trajectory is calculated through integration of the equation of the balance of forces acting on the particle. The equation describing the particle velocity, in the Lagrange formulation, for the $z$-component of Cartesian coordinate system has the form
\[
\frac{d u_p}{d t} = F_D(u - u_p) + \frac{g_z (\rho_p - \rho)}{\rho_p} + F_z,
\]
where \(u_p\) and \(u\) are the particle and air velocities, \(\rho_p\) and \(\rho\) are the particle and air densities, respectively, and \(g\) is the gravitational acceleration. \(F_z\) in Eq. (10) expresses the sum of the all external forces acting on the particle suspended in the air. For the purpose of this analyzes Brownian motion and Saffman’s lift force are considered. Details of components of Brownian force and Saffman’s lift force could be found in Ref. [8]. Here, \(F_D\) is the drag force calculated from the expression:

\[
F_D = \frac{18 \mu C_D \Re}{\rho_p d_p^2} 24 ,
\]
where \(\mu\) is the air viscosity, \(d_p\) is the particle diameter and the Reynolds number is defined as

\[
\Re = \frac{\rho d_p |u_p - u|}{\mu}.
\]

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

\[
C_D = a_1 + \frac{a_2}{\Re} + \frac{a_3}{\Re^2}
\]
where \(a_1, a_2, \) and \(a_3\) are constants that apply to smooth spherical particles over several ranges of \(Re\) number given by Morsi and Alexander [9].

3 RESULTS AND DISCUSSION

In general, breathing patterns are pulsatile in nature. However, Zhang et al. [10] have proposed a matching Reynolds number, i.e. an inlet Reynolds number \(Re_{match} \approx 0.5 \left(Re_{mean} + Re_{max}\right)\) representing the inhalation cycle. For the steady inhalation phase a uniform velocity profile calculated from matching Reynolds number is specified for the air at the inlet of G3 bronchi generation. The initial particle velocities are set equal to that of air. The boundary conditions for governing equations include symmetry with respect to the plane of the bifurcation, and no slip at the rigid impermeable walls. At the outlet uniform pressure condition is employed.

Figure 2 depicts the computed flow patterns in bronchial generations G3 through G6 at a constant resting inhalation rate of \(Q=15\) l/min. Flow field computations are only presented for \(k-\omega\) model for illustrative purposes. The remaining models employed in this work, i.e. standard and low Reynolds \(k-\varepsilon\) models, produce very similar flow patterns.

In Figure 3, the computed flow patterns in bronchial generations G3 through G6 at a constant moderate exercising inhalation rate of \(Q=60\) l/min are illustrated. Comparison of Figures 2 and 3 demonstrates strong dependency of flow fields on inhalation rate. It could also be noticed that downstream flow peaking becomes more pronounced as inhalation rate increases. Hence, it could be presumed that deposition hot spots of the inhaled aerosol particles will be relatively more concentrated around the midway of the first generation bronchi as bifurcation goes on.
For the particle trajectory and deposition pattern simulations through airway generations G3-G6, 18000 aerosol particles are injected at the inlet of G3. The distribution of these 18000 randomly injected particles follows the inlet velocity profile of the air. The 3-D views of the local particle deposition patterns in terms of number of particles deposited for particles with aerodynamic diameters 1 and 10 μm are shown in Figures 4 and 5, respectively. In both cases, computations are carried out with \( k-\omega \) model for resting inhalation conditions. Microparticle deposition during inhalation is mainly due to impaction, secondary flow convection, and turbulent dispersion. As a result, micron-size particles mainly accumulate at stagnation points for axial particle motion and the regions just upstream of the straight bronchi tube. The contribution of turbulent dispersion on deposition is stronger for small-size particles; say 1 μm, than for larger-size particles as seen from the figures. In Figures 6 and 7, similar to resting case, local deposition patterns of deposited particles with aerodynamic diameters 1 and 10 μm are shown for moderate exercise conditions. For large-size 10 μm particles at moderate exercise case, most of the deposition occurs in the first generation Bronchi G3 as seen from Figure 7. This could be attributed to the impaction and inertial effects which dominate over other forces acting on the aerosols.
Figure 4: Deposition patterns of 1 μm particles through bronchi generations G3-G6 at resting inhalation rate (Q=15 l/min) computed using $k - \omega$ model

Figure 5: Deposition patterns of 10 μm particles through bronchi generations G3-G6 at resting inhalation rate (Q=15 l/min) computed using $k - \omega$ model

Figure 6: Deposition patterns of 1 μm particles through bronchi generations G3-G6 at moderate exercise inhalation rate (Q=60 l/min) computed using $k - \omega$ model
The regional deposition of particles in human airways can be quantified in terms of deposition efficiency (DE) in a specific region (e.g., oral airway, first, second, and third bifurcation etc.). It is defined as the ratio of the number of deposited particles in a specific region to the number of the particles entering this region. Of interest are deposition efficiencies as well as deposition patterns from nano-size particles range (10 nm) to micro-size particles range (10 \(\mu\)m). Figures 8, 9, 10, 11, and 12 depict particle deposition efficiencies for bronchi generations G3 through G6 at resting and moderate exercising inhalation conditions for the specified range of particle aerodynamic diameters. Figure 8 illustrates DE values computed using \(k - \omega\) model. In Figures 9, 10, 11, and 12, DE values computed using Standard \(k - \varepsilon\) Model as well as some three of Low Reynolds Number \(k - \varepsilon\) Models (AB, AKN, CHC), respectively, are presented.

When the DE values of different models are compared in Figures 8-12, it becomes apparent that \(k - \omega\) model and low Reynolds number \(k - \varepsilon\) models apply equally well in particle deposition computations. Results of low Reynolds number \(k - \varepsilon\) models as well as \(k - \omega\) model are found in perfect agreement with the results of Ref. [11]. Standard \(k - \varepsilon\) model DE values considerably differ from the results of other models and it seems not a suitable model for particle deposition computations in tracheal bifurcations.

Figure 7: Deposition patterns of 10 \(\mu\)m particles through bronchi generations G3-G6 at moderate exercise inhalation rate (\(Q=15\) l/min) computed using \(k - \omega\) model

Figure 8: Deposition efficiency (DE) vs. particle diameter in \(k - \omega\) turbulence model.
Figure 9: Deposition efficiency (DE) vs. particle diameter in standard $k-\varepsilon$ turbulence model.

Figure 10: Deposition efficiency (DE) vs. particle diameter in low Reynolds number AB $k-\varepsilon$ turbulence model.

Figure 11: Deposition efficiency (DE) vs. particle diameter in low Reynolds number AKN $k-\varepsilon$ turbulence model.
CONCLUSIONS

It is observed that deposition patterns in tracheal bifurcations are not very sensitive to the particle size for small micron size particles at low inhalation rates. Major deposition mechanism during inhalation of small size micron and nano-particles is demonstrated to be diffusion at the tracheal walls which allows penetration of aerosols to the further trachea. At high inhalation rates, impaction is observed to become more pronounced especially for large aerodynamic diameter aerosol particles; as a result, most of the particles are deposited in the main airway generation. Hot spots of deposition mostly occur in the vicinity of carinal ridge and at the inner sides of the daughter airways downstream of the carina.

It is shown that $k-\omega$ and low Reynolds number $k-\varepsilon$ models of FLUENT such as AB, AKN and CHC produce results which are in perfect agreement among themselves and with the literature for particle deposition computations. It is also shown that standard $k-\varepsilon$ model is not suitable for analysing aerosols deposition in human respiratory system.

Considering the fact that the dose distribution due to the deposited particles in lungs rather than its average value is more crucial, it is demonstrated in this work CFPD simulations are very convenient tools to estimate local depositions of radioactive aerosols. Based on the deposition calculations presented in the current study, local dose distribution in lungs due to radioactive particles intake could be determined as a further step which will be the subject of our next study.

REFERENCES


