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Airflow dynamic and particle deposition in age-specific human lungs

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Abstract

Particle transportation and deposition (TD) during inhalation drug delivery in human lungs is affected by lung anatomy, breathing pattern, as well as particles properties. The lung volume and breathing capacity reduce as age increases. It is found that diameters of lung airways reduce by about 10% after every 10-years for over 50-year age people. However, the studies on the particle TD in age-specific human lungs are still very limited in the literature. Therefore, it is important to understand the effects of aging on targeted drug particle deposition. In this study, numerical simulations are conducted to investigate the particle TD in human lungs for people of 50 to 80-year ages. The ANSYS FLUENT solver based on the finite volume discretization method is used for numerical calculations. The variation of inhalation rates and lung diameters with age is considered. The results show that the deposition efficiency of old age people is higher than that of young age people. Moreover, the majority of the particles are deposited in the first bifurcation area of lungs of the 50-80 year ages at generation G9-G13.

Keywords

Ageing effect, Airflow, Aerosol particle transport and deposition (TD). Lung, Inhalation, Drug delivery.

1. Introduction

Many old people who suffer from lung diseases such as pneumonia, Chronic obstructive pulmonary disease (COPD), and asthma need mechanical ventilation to improve the breathing condition. Mechanical ventilation is use of a machine to aid the movement of air into and out of the lungs. The average death rate of patients on mechanical ventilation is 35%, and it is 53% for old age people Kim, Heise [1]. In addition, mechanical ventilation may cause lung injury. Therefore, age-specific modelling of aerosol particle transport and deposition in a human lung is useful for the treatment of lung diseases in the respiratory tract, mainly because the lung volume and breathing capacity reduces as age increases. The research outcome based on young lungs does not apply to old ages people [2].

The deposition efficiency is defined as the percentage of aerosol particles absorbed in the human lung airways. The aerosol particle deposition efficiency of teenagers changes fast because of the fast growth rate of the lungs. Xu and Yu [3] developed a theoretical model for predicting the deposition of inhaled aerosol in the respiratory tracts of young ages ranging from newborn babies to adults. The results showed that the deposition efficiency in the mouth-throat region of children is higher than the adults. However, in the pulmonary and alveolar region, the opposite results are found due to the ageing effect [4, 5]. Kim, Heise [1] studied the airflow dynamics of Weibel's based symmetric lung models of old age people. It was found that the vacuum pressure of lung airways of 80-year-old people decreases by about 38% than 50-year-old. However, the authors did not consider the particle deposition. Deng, Ou [6] studied the particles deposition in human lungs of three age groups: infant, child, and adult through numerical simulation. They found that the deposition efficiency in the tracheobronchial region of children is higher than adults. Their study is important for the healthy growth of infants and children. However, most of the drug was prescribed for old age people. Therefore, it is important to understand and improve particles deposition efficiency in the lungs of old age people. Recently, CFD has become an efficient and effective method for predicting the mechanisms of the local particles deposition pattern [7, 8].

This study is aimed to understand the flow characteristics and quantify the particle deposition efficiency in symmetric lung models of older 50-80-year age people through CFD simulations. The effect of particle size on the deposition efficiency is also quantified.

2. Lung Model

2.1. Lung Geometry

The number of division of trachea is called generation (G). A three-dimensional (3D) symmetric model from generation G9 to G13 is constructed based on Xu and Yu [3]. The diameters of lung airways do not change for fully grown people between the ages of 30 to 50 [9]. Therefore, we have assumed that the diameters and lengths of lung airways of 30-year-old people are the same as their counterparts of 50-year-old people. However, the airway diameters reduce by 10% after every 10 years if the age is above 50 [1, 10].

The SolidWorks software is used to generate lung airways of 50-year of age shown in Figure 1. The lung models of 60, 70, and 80 year of age are generated by reducing the diameters of airways by 10% after every 10 years. The ANSYS FLUENT solver is used for the computational purpose, and Tec-plot software is used for visualization of particles deposition in the lung airways.

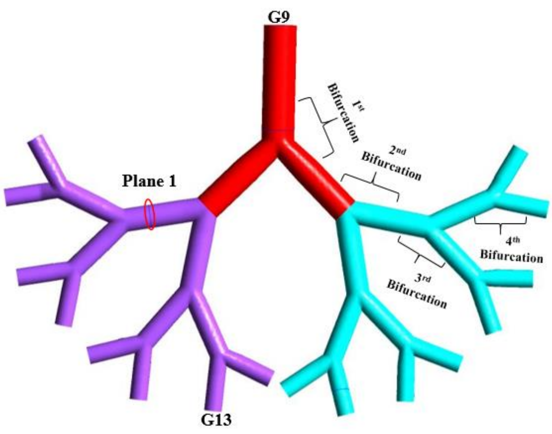
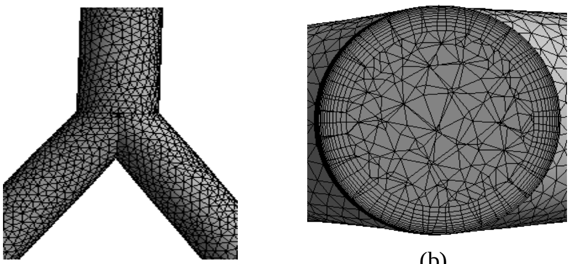


Figure 1. Tracheobronchial lung airways model (G9-G13) of the 50-year age

2.2. Mesh generation

The geometric parameters of the lung airways are listed in Table 1. Ten layers smooth inflation is implemented near the wall to accurately predict the near-wall boundary flow inside lung airway in Figure 2(b).



(a) (b)

Figure 2. (a) The mesh of lung airway, (b) Refined inflation mesh near the airway wall

Table 1 The parameters of lung airways

Generation (G)	Diameter (cm)				Length (cm)
	50 year	60 year	70 year	80 year	50-80 years
9	0.154	0.139	0.123	0.108	0.538
10	0.129	0.117	0.104	0.091	0.460
11	0.109	0.098	0.087	0.076	0.390
12	0.095	0.085	0.076	0.067	0.330
13	0.082	0.074	0.066	0.057	0.271

3. Numerical method

3.1. Airflow Model

The fluid flow is simulated by solving the momentum equation and the continuity equation;

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \quad (1)$$

$$\frac{\partial}{\partial t}(\rho \vec{u}) + \nabla \cdot (\rho \vec{u}\vec{u}) = -\nabla p + \nabla \cdot \left(\mu\left[(\nabla \vec{u} + \nabla \vec{u}^{T}) \quad - \frac{2}{3}\nabla \cdot \vec{u}I\right]\right) + \rho \vec{g} \quad (2)$$

where $\vec{u}$ is the fluid velocity, μ is the dynamic viscosity of the fluid, I is the unit tension, ρ is the fluid density, p is the pressure, $\vec{g}$ is the gravitational acceleration, $\rho\vec{g}$ is the body force based on gravity.

The second-order upwind numerical scheme [11] is considered to simulate the discrete phase. The coupling algorithm [12] has been used for the pressure-velocity coupling scheme.

3.2. Particle transport and deposition model

The Lagrangian approach is applied to simulate the particle transport in human lung airways. Therefore, the force balance equation based on the Newtons second law is used to calculate the particle motion:

$$\frac{d\vec{u}_p}{dt} = F_D\left(\vec{u} - \vec{u}_p\right) + \frac{\vec{g}}{\rho_p}\left(\rho_p - \rho\right) + \vec{F} \quad (3)$$

where $\vec{u}$ represents fluid velocity, $\vec{u}_p$ represents the aerosol particle velocity, $\vec{g}$ represents the gravitational acceleration, ρ_P is the particle density, $\vec{F}$ represents the additional acceleration force term with is set zero ($\vec{F} = 0$). $F_D\left(\vec{u} - \vec{u}_p\right)$ is the drag force per unit particle mass, and the coefficient F_D is calculated by;

$$F_D = \frac{18\mu}{\rho_p d_p^2} C_D \frac{Re_P}{24} \quad (4)$$

where C_D is the drag coefficient. The drag coefficient for the spherical particles can be represented by:

$$C_D = a_1 + \frac{a_2}{Re_P} + \frac{a_3}{{Re_P}^2}$$

where a_1, a_2, a_3 are constants that apply over several ranges of Re_P given by Morsi and Alexander [13].

$$a_1, a_2, a_3 = \begin{cases} 0, \quad 24, \quad 0 & 0 < R_e < 0.1 \\ 3.690, \quad 22.73, \quad 0.0903 & 0.1 < R_e < 1 \\ 1.222, \quad 29.17, \quad 3.89 & 1 < R_e < 10 \\ 0.617, 46.50, -116.67 & 10 < R_e < 100 \\ 0.364, 98.33, -2778 & 100 < R_e < 1000 \\ 0.357, 148.62, -47500 & 1000 < R_e < 5000 \\ 0.46, -490.546, 578700 & 5000 < R_e < 10000 \\ 0.519, -1662.5, \quad 5416700 & R_e > 10000 \end{cases}$$

The Reynolds number (Re_P) is the ratio of inertial forces to viscous forces, and it can be defined as:

$$Re_P = \rho d_P \left|\vec{u}_p - \vec{u}\right| / \mu.$$

The maximum Reynolds number of the current studies is 164.33. The laminar flow model has been considered during the simulation.

The pressure outlet and velocity inlet boundary conditions are considered in the lung airway model for generation G9-G13. The zero-pressure condition was used on all the outlets of the lung model. In each simulation, spherical particles with uniform size were injected randomly from the inlet surface. Totally 26000 particles are injected from the inlet surface at one time. The particles density is 1100 kg/m^3 [14]. A 'trap' condition is considered in the airway walls for particles deposition, and an escape condition is considered at the outlets [6, 15]. More specifically, the coefficient of restitution is zero because of the trap condition; therefore, no bounce happens when the particles are touching the lung airways surface. If a particle touches the lung wall surface, which is sticky in reality, it is trapped and stay on the surface because of the trap condition.

3.3. Deposition Efficiency calculation

The deposition efficiency (η_d) is the percentages of the particles absorbed (trapped) in the human lung airways. It is calculated by:

$$\eta_d = \frac{\text{Number of particles are trapped in a lung airways}}{\text{Total number of particles released in the lung airways}}$$

4. Results and discussion

4.1. Grid refinement test

The grid refinement test conducted to ensure the converged solutions are obtained. Simulations are conducted using six meshes with different densities. The average velocity magnitude measured on plane 1, indicated in Figure 1 as a function of the number of grid elements is shown in Figure 3. It can be seen that the velocity changes little after the number of elements is 0.53 million and above. Therefore, we used the mesh with 0.53 million elements for all the rest of the simulations.

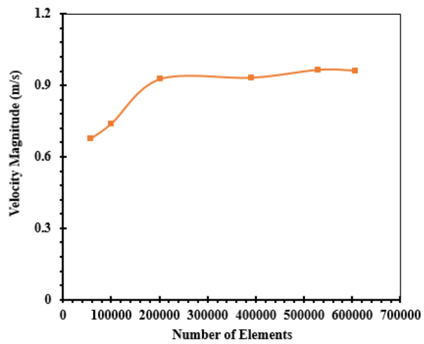
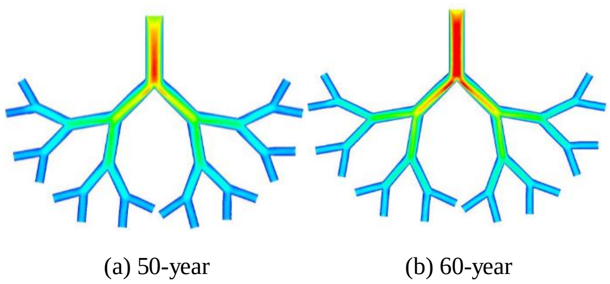


Figure 3. The average velocity measured at plane-1 indicated in Figure 1

4.2. Airflow analysis

A constant airflow flow rate of $Q_{in} = 60\,\mathrm{l/min}$ at the first-generation G0 is considered. However, the number of airway branches of the nth generation is 2^n, where n is the generation number. Therefore, the flow rate at the generation G9 is $Q_{in} = 0.12\,\mathrm{l/min}$, the flow rate at G0 divided by 2^n. The distribution of the airflow velocity magnitude of four lung models is shown in Figure 4. The airflow velocity is increased with the increase of the age because the airway diameters decreases. The highest velocity is observed in the upper part of the lung of the 80-year age.



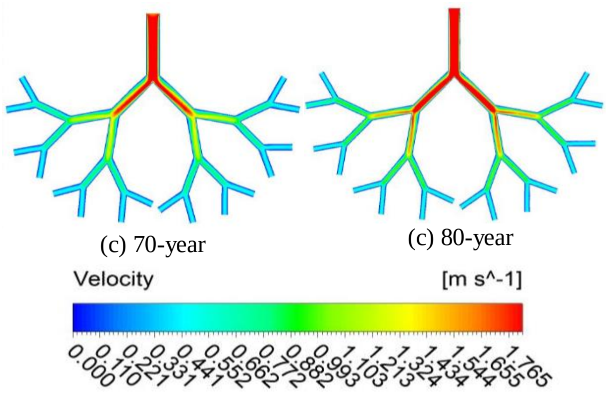


Figure 4: Velocity magnitude of lung models at four ages.

4.3. Particle Deposition

The total particles deposition rates within the lung airways at the flow rate of $Q_{in} = 0.12\,\mathrm{l/min}$ are shown in Figure 5. The total deposition rate (η_d) is significantly affected by the particle diameter. Small particles usually follow the airflow streamlines [16]. However, the large particles do not follow streamline at positions where the flow velocity changes its direction. Therefore, the deposition rate increases with the increase of the particle diameter. The inertia effect makes large particles travel with its original track when the airway bends and hit the inner wall of airways. This mechanism of deposition is the typical impaction mechanism.

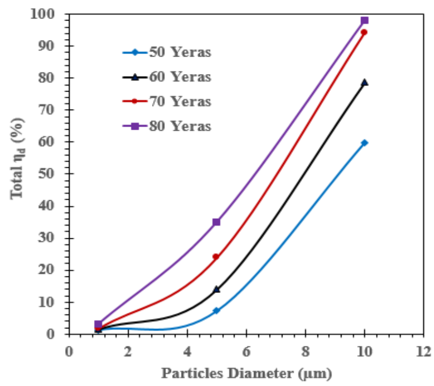
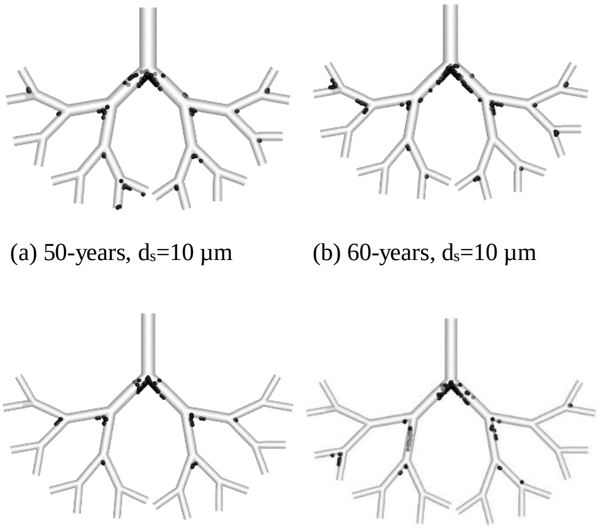


Figure 5. Total Deposition Efficiency as a function of particles diameter for 50-80 years' lung model

It is proved that ages affect the deposition rate. At the flow rate of $0.12\,\mathrm{l/min}$ at G9, the total deposition rates of the lung models of 50, 60, 70 and 80-year ages are 59.89%, 78.71%, 94.3 % and 98.15%, respectively. The deposition rate is increased with the increase of age as shown in Figure 5. Moreover, around 2% of 1 µm size particles are deposited in the whole lung model. The variation trend of total deposition rate with particle diameter is in good agreement with that found in reference [17].

Figure 6 shows the visualization of the distribution of particles with 10 µm diameter in four lung models. The deposition efficiency for the 80 years old age is the highest. Most of the particles are deposited in the first bifurcation area.



(a) 50-years, d_s=10 µm (b) 60-years, d_s=10 µm

(c) 70-years, d_s=10 µm (c) 80-years, d_s=10 µm

Figure 6. Particles deposition of 10 µm particles at a flow rate of 0.12 l/min at inlet for 50-80 year age models

Conclusion

The micro-particle TD in the generation G9-G13 lung airways is simulated through CFD simulations. The effects of the particles size and age on the deposition efficiency are studied. The deposition efficiency increases with the increase of particle size. The deposition efficiency of old age people is higher than that of young age people because the diameter of the lung is reduced. The results will help to understand the deposition efficiency for different size particles as targeted drug delivery lung airways of old age people. Only inhalation condition was considered in the simulation of airflow dynamic and particles deposition. The dynamic wall motion was not considered during this study. More bifurcation branches up to 23 generations will be considered in future studies.

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