Study on airflow and inhaled particle deposition within realistic human upper respiratory tract

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Abstract. Based on the CT (Computerized Tomography) scanned images of a 19-years-old healthy boy, a realistic geometric model of URT from nasal cavity to the upper six-generation bronchial is rebuilt. To investigate airflow and particle deposition in the obtained realistic human upper respiratory tract, RNG k-ε turbulence model was used to describe the primary flow and particle deposition under three breathing intensity such as 15 L/min, 30 L/min and 60 L/min. The particle is tracked and analyzed in the Lagrangian frame. The velocity fields of airflow under different airflow rates were computed and discussed. The trapping of particles with diameter 1μm on the wall surfaces was monitored, and the locations of trapping in different region were visualized.

In order to study the characteristics of particles movement and the effect of particles diameter on the deposition pattern, eleven kinds of sphere particles with different diameters are selected as research object. The diameters of selected particles as follows: 0.1μm, 0.5μm, 1μm, 2.5μm, 3μm, 3.5μm, 4μm, 4.5μm, 5μm, 6.5μm and 8μm. The variation of inhalable particles deposition in realistic human upper respiratory tract with respiratory intensity and particle size was researched and compared.

1. INTRODUCTION

Particles ranging from toxic particulate matter to drug aerosols may be inhaled into people’s respiratory tract, and some of them can be either harmful or therapeutic to humans depending upon the aerosol material, deposition site and local concentration. In turn, these aspects and parameters are greatly determined by the airflow field, particle properties, breathing pattern and geometric airway characteristics. Thus, good knowledge of airflow structure, deposition of particles in the upper respiratory tract can provide credible theoretical foundation not only for preventing illness of respiratory tract effectively. On the other hand, it is desirable to deliver pharmaceutical aerosols to the targeted part accurately, and thus effectively reduce drug dosage and pain of patients (Balásházy et al., 2003).

Hitherto, especially in the last decade, many research literatures about computation fluid dynamics modeling of airflow and particles movement in the respiratory tract are available all over the world. Most models employ low-Reynolds k-ω model and standard k-ε model to describe gas flow,
track particles movement in the frame of Lagrange. Using a mouth-to-trachea replica plus three generations of the Weibel A bronchia, Zhang et al. (2005) as well as Zhang et al. (2006) investigated numerically steady inhaled particle transport and deposition. Employing a Weibel-type bifurcation and considering chronic obstructive pulmonary disease (COPD), Yang et al. (2006) and Liu et al. (2003) compared the resulting airflow structures under different inlet conditions. Tang et al. (2004) presents a brief summary of flow features in the human respiratory system and simulates an airflow field based on a 3D real-anatomical geometry of the human nasal cavity. The dispersed phase in the flow field is solved by Lagrangian particle-tracking approach. Hofmann et al. (2001) computed the inspiratory deposition efficiencies of ultrafine particles with 6500 nm in airway Generations 3 and 4 for different inlet flow rates. Just recently, the LES method is employed to the study of airflow in the human respiratory tract (Jin et al., 2007). For the geometric model, it can be found that most simulation is based on the idealized, i.e., planar and symmetric, lung airway model published by Weibel (1963). Recently, modern imaging techniques allowed for even more detailed mapping of the human respiratory system (Cebral and Summer, 2004). CFD simulations based on the CT scanned images are conducted (Xi and Longest, 2007; Shi et al., 2007). Nowak et al. (2003) conducted computational fluid dynamics (CFD) simulations of airflow and particle deposition in geometries representing the human tracheobronchial tree. Two geometries were used in this work; one of them is based on a CT scan of a cadaver lung cast. Flow conditions used included both steady-state inhalation and exhalation conditions as well as time-dependent breathing cycles. Particle trajectories were calculated in each of these models by solving the equations of motion of the particle for the deterministic portion of particle displacement. The trapping of particles on the wall surfaces was monitored, and the locations of trapping in each generation were recorded.

The objectives of this paper is to rebuilt a three-dimensional geometric model of realistic human upper respiratory tract including nasal cavity, pharynx, larynx, trachea and the upper six-generation bronchial based on the CT scanned images. On the other hand, RNG k-ε turbulence model is employed to study the airflow and particles deposition in this realistic human upper respiratory tract.

2. DESCRIPTION OF MATHEMATICAL MODEL

2.1 Geometric model

Transverse CT images were obtained from a healthy 19-year-old normal adult male (the volunteer was awake and reclining). The subsequent CT images were then transferred to a 3-dimensional structure of the airway by image and graphics recognition technologies. The obtained 3-dimension upper airway is shown in figure 1. The geometric structure of the upper airway is very complex, especially the nasal cavity, which is different from most previous model. This will cause complicated airflow fields in the upper airway, and complicated particle transport and deposition principles along the airway. The more real flow characteristics can be obtained using this realistic geometrical model.
The airflow structure will be very complex because sharp shrink and expand segment exist in the pharynx-larynx, bifurcate structure exist in the bronchia and the nasal cavity with more complex structure. Thus, the RNG $\varepsilon-k$ turbulent model is adopted in this paper, which provides an option to account for the effects of swirl or rotation by modifying the turbulent viscosity appropriately. Furthermore the RNG $k-\varepsilon$ model is more responsive to the effects of rapid strain and streamlines curvature than the standard $k-\varepsilon$ model. The continuity and movement equations:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0 \quad (1)$$

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial^2 u_j}{\partial x_j \partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] + \rho g_i \quad (2)$$

The turbulence kinetic energy, $k$, and its rate of dissipation, $\varepsilon$, are obtained from the following transport equations:

$$\frac{\partial (\rho k)}{\partial t} + \frac{\partial (\rho k u_i)}{\partial x_i} = \frac{\partial}{\partial x_j} \left( \alpha_k \mu_{eff} \frac{\partial k}{\partial x_j} \right) + G_k + \rho \varepsilon \quad (3)$$

$$\frac{\partial (\rho \varepsilon)}{\partial t} + \frac{\partial (\rho \varepsilon u_i)}{\partial x_i} = \frac{\partial}{\partial x_j} \left( \alpha_\varepsilon \mu_{eff} \frac{\partial \varepsilon}{\partial x_j} \right) + \frac{C_{1e}}{k} \frac{\varepsilon}{k} G_k - \frac{C_{2e}}{k} \rho \frac{\varepsilon^2}{k} \quad (4)$$
\[ \mu_{\text{eff}} = \mu + \mu_t; \mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \]
\[ C_{1e} = C_{1e}^* = \frac{\eta(1-\eta/\eta_0)}{1 + \beta \eta^2}; \eta = (2E_{ij} \cdot E_{ij})^{1/2} \frac{k}{\varepsilon}, \]
\[ E_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \]

Where \( i, j = \{1, 2, 3\} \), \( \rho \) is fluid density, \( t \) is time, \( u \) is fluid velocity vector, \( x \) denotes the spatial coordinate, \( p \) stands for average pressure, \( \mu \) is fluid viscosity, \( \mu_t \) is turbulent viscosity, \( g_i \) is the gravity in the \( i \) direction, \( k \) is turbulence kinetic energy, \( \varepsilon \) is turbulence dissipation rate, \( G_k \) represents the generation of turbulence kinetic energy due to the mean velocity gradients, The quantities \( \alpha_k \) and \( \alpha_\varepsilon \) are the inverse effective Prandtl numbers for \( k \) and \( \varepsilon \), \( \beta \) is thermal expansion coefficient, \( E_{ij} \) implies main time-average strain rate. \( C_\mu \) and \( \eta_0 \) are model constants. The model constants \( C_{1e} \) and \( C_{2\varepsilon} \) have values derived analytically by the RNG theory.

The particle phase in the air can be considered as dilute phase, and neglecting the interaction between particles. The Lagrangian dispersed phase model is used for the prediction of the trajectory of a particle. This is done by integrating the force balance on the particle. In a Lagrangian reference frame, movement vector of a single particle can be written as:
\[ m_p \frac{dv_i}{dt} = F_{\text{particle}} = m_p g_i \delta_d - \frac{1}{2} \rho \frac{d}{d_x} u_i - \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \]

Where, \( m_p \) is particle mass, \( d_p \) is particle diameter, \( v_i \) represents particle velocity vector, \( C_D \) stands for particle resistance coefficient, \( g \) acceleration of gravity. The three terms on the right hand are Stokes resistance, gravity force and Saffman’s lift force respectively, which are considered in this paper.

The particle deposit efficiency (DE) is introduced to quantificationally analyze particle deposit in different region of the respiratory tract:
\[ \text{DE} = \frac{N_d}{N_t} \times 100\% \]

Where \( N_d \) denotes the number of particle deposited on wall of some region in the respiratory tract, \( N_t \) represents the total number of particle inhaled into the model.

2.3 Initial condition and boundary condition

First of all, three-cycle pre-simulation are conducted to eliminate initial effect because the inlet velocity is stable during stable breath. The pressure outlet boundary is imposed on the outlet of bronchial, i.e., the pressure is zero and gradient of other variables is zero. When the particles impact
with model wall, it is marked as deposition and the track computation is over, which accords with the real instance well. Different from many papers, the pressure inlet condition is selected for the computation of this paper. One box extending from nasal inlet is added to consider the inlet effect because the pressure at nasal inlet is not equal one atmosphere but the boundary of the box.

### 3. RESULTS AND DISCUSSIONS

#### 3.1 Gas phase

Three breathing intensities $Q=15\text{L/min}$, $Q=30\text{L/min}$, $Q=60\text{L/min}$ are computed respectively.

Figure 2 depicts the typical velocity vectors and pressure contours during inhalation phase for the airflow rate $Q=15\text{L/min}$. The outside air is inhaled into nasal cavity by the pressure difference between interior lung and outer circumstance. The air stream arrive a relatively high velocity after entering the nasal cavity due to the constrictive structure in the inlet segment. At the cross-section A-A (Figure 2a), the maximum velocity is located at the lower wall when airflow through the syphon structure. Then the velocity value decrease from the lower wall to the upper wall till little-value reverse velocity appears close to the upper wall. Corresponding to Figure 6b, we can find that the domain with reverse velocity is the negative pressure region, which is the first negative pressure region after the gas stream entering the nasal cavity and there exists one relatively faint vortex. After the syphon structure, the maximum velocity value of gas stream is gradually transferred to the upper wall of olfactory airway of nasal cavity, which is directly eroded by gas stream. The possibility of particle deposition in the vortex region is very low for the low velocity in this domain. However the particle is prone to deposit at the upper wall of syphon structure and partial olfactory airway behind that.

![Velocity vector at selected cross-sections](image1.png) ![Pressure contours in the right nasal cavity in the nasal cavity](image2.png)

**Fig.2** The typical velocity vectors and pressure contours during inhalation phase for the airflow rate $Q=15\text{L/min}$

Figure 3 illustrates the velocity contours in the pharynx-larynx part and bronchia bifurcation for breath intensity $Q=60\text{L/min}$ during inhalation phase. The maximum velocity of the whole model with $V_{\text{max}}=3.82 \text{m/s}$ lies in the pharynx. There has one shrink structure in the larynx; the maximum velocity at the cross-section in the larynx exhibits close to the posterior wall. After entering into bronchia, the maximum velocity at the cross-section in the bronchia gradually moves towards the center of the tube, and the gradient of pressure and velocity is small. The velocity of bifurcation is plotted in figure 3b. It can be seen from figure that the gas stream erodes the carinal ridge directly, the carinal ridge of every generation bronchia and its daughter tube will be the hot spot for particles deposition.
(a) Velocity contours in the pharynx-larynx

(b) Velocity contours in the bronchia bifurcation

Fig. 3 Velocity contours in the pharynx-larynx and bronchia bifurcation for breath intensity $Q=60\text{L/min}$ during inhalation phase

(a) E-E

(b) F-F

(c) G-G

(d) H-H

Fig. 4 Secondary velocity vectors at selected cross-sections in the nasal cavity during exhalation phase for the breath intensity $Q=15\text{L/min}$
Figure 4 plots the velocity vectors at selected cross-sections in the second half nasal cavity with breath intensity $Q=15\text{L/min}$ during exhalation phase. It is different from inhalation process that the maximum velocity is located at the center of section and there have two distinct and symmetry vortex in both sides of the section when the gas stream flows through section H-H. Then, when the gas stream flows through the G-G and F-F section, the vortexes in two sides of section move towards center, the maximum value of velocity at the center position decrease gradually and the corresponding velocity gradient. After that, when the gas stream flows through the E-E section, around which the gas stream is divided into the left and right nasal channels, the vortexes disappear.

3.2 Particles deposition

3.2.1 Map of particle deposition

Fig. 5 Particles deposition in different part of the respiratory tract with $d=1\mu\text{m}$ and $Q=15\text{ L/min}$ during inhalation phase, the darkish particle indicates deposition at the rear wall.
In order to investigate the particle deposition position and hot spots, Lagrange method is implied to track the particle movement. The particle deposition at different parts and under different breath intensities are visualized in figure 5. The figure a plots the deposition in the bronchia, from which we can see that the particle preferred deposition in the carinal ridge and downstream at the inner tube of the daughter tubes for the effect of impact between particle and wall. The deposition in the nasal cavity, pharynx-larynx, and trachea is shown in figure. It can be seen from figure that the deposition in the front of the pharynx-larynx is small for the air flow affected by the geometry structure.

The deposition efficiencies of particle with diameter 1μm in the different parts under different breath intensities are plotted in Figure 6. It can be seen from figure that the total deposition efficiency in the whole model slackly increases as the breath intensity increases. The deposition efficiency in the nasal cavity decreases as the breath intensity increases; however, the deposition efficiency in the pharynx-larynx, trachea and bronchia slackly increases as the breath intensity increases. Among all the parts, the deposition efficiency in the nasal cavity is the largest; almost half particle is deposited in this region. The next sequence of deposition efficiency is bronchia, pharynx-larynx and trachea. The deposition efficiency in the trachea is the smallest for the relatively smooth tube structure in the trachea position.

![Deposition Efficiency Chart](image)

**Fig. 6 Numerically predicted total and regional deposition efficiencies of 1 μm diameter particles under three breath intensities**

### 3.2.2 Variations of deposition rate with inhaled particles diameter and airflow rate

In order to study the effect of particles diameter and airflow rate on the deposition characteristics, eleven kinds of monodisperse particles with diameter 0.1μm, 0.5μm, 1μm, 2.5μm, 3μm, 3.5μm, 4μm, 4.5μm, 5μm, 6.5μm, 8μm and three airflow rates Q=15, 30 and 60L/min are simulated.

The variation of total particles deposition rate in the whole model with breath intensity is illustrated in figure 7. For the breath intensity with 15 L/min, the deposition rate faintly decreases as increase of the diameter smaller than 6.5μm, increase as increase of the diameter larger than 6.5μm. For the breath intensity with 30 L/min, the deposition rate decreases as increase of the diameter which is smaller than 4μm and increases as increase of the diameter which is larger than 4μm. For the breath intensity 60 L/min, the deposition rate decreases as increase of the diameter smaller than 2.5μm, and
increase as increase of the diameter which is larger than 2.5 μm. The deposition in the nasal cavity occupies more than half deposition in the whole model and directly determines the total deposition characteristics. Be similar to the deposition rate in the nasal cavity, the diameter corresponding to the minimum deposition transfers towards small size as the breath intensity increase.

![Fig. 7 Variation of total particles deposition rate in the whole computation domain with breath intensity](image)

4. CONCLUSIONS

A three-dimension geometric model of a real human upper respiratory tract including nasal cavity, pharynx, larynx, trachea and upper six generations bronchial based on the CT scanned images is rebuilt in this paper. RNG k-ε turbulence model is used to compute airflow, particle movement and deposition efficiency in the obtained complex structure geometrical model. The three-dimensional flow structure under three different breathing intensity are computed and analyzed. Then particle of 1 μm diameter in every part of respiratory tract are tracked and visualized under Lagrange frame. The result indicates that the total deposition efficiency in the whole model slackly increases as the increase of breathing intensity. The deposition efficiency of different particles with diameter 0.1 μm, 0.5 μm, 1 μm, 2.5 μm, 3 μm, 3.5 μm, 4 μm, 4.5 μm, 5 μm, 6.5 μm, 8 μm in the realistic human respiratory tract is simulated in this paper.

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