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Numerical study of the airflow structures in an idealized mouth-throat under light and heavy breathing intensities using large eddy simulation

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ABSTRACT

An excellent understanding of the airflow structures is critical to enhance the efficiency of drug delivery via the human oral airway. The present paper investigates the characteristics of both steady and unsteady airflow structures in an idealized mouth-throat using large eddy simulation (LES). Representative inhalation flow rates of 15 L/min at rest and 60 L/min in exercise are considered. The study shows that there are more secondary vortices in the pharynx and the laryngeal jet is much longer and more concave in the steady flow field at 15 L/min compared to the higher inspiration rate, which decreases the possibility of drug impinging on the wall. In contrast, the laryngeal jet is much more unsteady at heavy breathing and its strong interaction with the recirculation zone in the trachea leads to a enlarged mixing zone, increasing the possibility for carrying the particles from the laryngeal jet into the recirculation zone, which will lead to a longer residence time of the particles in the trachea and this increases the possibility of drug deposition in this area. In addition, the recirculation zone size is larger, the separation region is far away from glottis, and the reversed flow is slower at light compared to heavy breathing. In conclusion, these airflow structures show distinct properties at light and heavy breathing conditions, particularly in the unsteady flow field. The study provides evidence about the physical processes leading to both enlarged mixing zones and recirculation zones. It is known that stronger secondary vortices, a stronger laryngeal jet and enlarged recirculation zones definitely increase the particle deposition in the upper airway. The present paper aims to uncover the physical properties of the airflow for different breathing conditions, and their detailed effect on particle deposition will be studied in future.

1. Introduction

Aerosol drug therapy, in which the drug mainly delivered through the nasal or oral airway to the lung or some other location of the respiratory tract, has become a popular way to treat different diseases such as asthma and chronic obstructive pulmonary disease, due to its advantage of smaller dosages, minimal systemic adverse effects and rapid response (Kleinstreuer et al., 2008). It is expected that such drugs can be controlled to reach special locations such as the position of a possibly existing tumor so that the drug is efficiently positioned and side effects are minimized. However, about 80–90% of the aerosol drug is filtered out in this region (Koullapis et al., 2016) and does not reach the lung. Enhancing the drug delivery efficiency requires an excellent understanding of the airflow field, which regulates the particle transport and deposition (Kleinstreuer et al., 2008).

The numerical modeling of airflow in the upper airway may be carried out based on different types of geometrical models such as idealized configurations (Zhang et al., 2002; Longest et al., 2009) and more realistic geometries generated from medical images (Mylavarapu et al., 2013; Mihaescu et al., 2011; van der Velden et al., 2016), which mainly consider the specific geometrical properties of the airway tract. The idealized geometry has the advantage of gaining common properties of the flow field in the upper airway across populations and it is widely used for the investigation of properties of the airflow structures in the upper human airway (Zhang and Kleinstreuer, 2011; Nicolaou and Zaki, 2016).

Moreover, various mathematical models that differ in the closure of the turbulent fluctuations of the flow field such as RANS (Reynolds-averaged Navier–Stokes equations) (Li et al., 2016), LES (large eddy simulation) (Jayaraju et al., 2008) and DNS (direct numerical simulation) (Nicolaou and Zaki, 2013; Stylianou et al., 2016), which resolves all turbulent length scales. In the present situation, LES is preferred over RANS and DNS. First of all, LES is superior to RANS in the transitional low Reynolds number regime (Koullapis et al., 2016; Stylianou et al.,

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2016; Cui and Gutheil, 2011). It has been shown that LES predicts the velocity profile better than RANS in the transitional flow region after the glottis of a constricted tube if compared with measurements (Cui and Gutheil, 2011). Comparing the cost of LES with DNS with respect to the computational time and physical resources, LES is much more economic and efficient (Jayaraju et al., 2008; Stylianou et al., 2016). Moreover, LES is capable of describing both the steady and unsteady flow fields (Jayaraju et al., 2008; Vaish et al., 2016). A brief review may be given as follows. The counter-rotating secondary vortices have been investigated in a widely used idealized mouth-throat using the LRN (low Reynolds number) k–ω model by Kleinstreuer and Zhang (2003). The unsteady properties of airflow structures are not discussed due to the limitations of the RANS approach. Cui and Gutheil (2011) investigated the unsteadiness of secondary vortices at a normal breathing condition of 30 L/min using LES, but they did not study the airflow field at light and heavy breathing conditions and no comparison with airflow structures at other inspiration flow rates was conducted. The characteristics of the laryngeal jet and recirculation zone have been addressed in several investigations (Longest et al., 2008; Pollard et al., 2008; Lin et al., 2007; Jayaraju et al., 2008; Fan et al., 2007; Yousefi et al., 2015; Li et al., 2016), but they mainly concern the two-dimensional cut plane, and three-dimensional properties were not sufficiently addressed. Moreover, the unsteady dynamics of secondary vortices was not studied and the laryngeal jet and the recirculation zone at light and heavy breathing in the widely used idealized mouth-throat geometry reported by Kleinstreuer and Zhang (2003) were not presented.

The present study focuses on the properties of the airflow structures including secondary vortices, recirculation zones and the laryngeal jet in both the steady and unsteady flow fields under light and heavy breathing of 15 L/min and 60 L/min, respectively, using large eddy simulation.

2. Configuration, mathematical formulation and solution procedure

2.1. Geometrical configuration

An idealized oral airway was built based on the human cast (Cheng et al., 1999) as shown in Fig. 1 (Kleinstreuer and Zhang, 2003). This model geometry has a variable circular cross-section, where the oral cavity-pharynx-larynx region is simplified as a nearly 180° curved bend as suggested by Cheng et al. (1999). The varied diameter at each cross section along the oral cavity towards the trachea is computed from the hydraulic diameters from a human oral airway cast of a healthy male adult with a half-open mouth (Kleinstreuer and Zhang, 2003; Cheng et al., 1999). At the mouth inlet, it is extended by a circular tube of 2 cm in diameter (Kleinstreuer and Zhang, 2003; Cui and Gutheil, 2011). The cross sections are also circular with a narrowed airway after the soft palate and in the glottis. Details are provided by Kleinstreuer and Zhang (2003) and Cui and Gutheil (2011). Special characteristics of that configuration is the sudden change of the flow direction that appears in the pharynx and the constriction of the airway at both the soft palate and the glottis.

2.2. Governing equations

Three-dimensional incompressible Navier–Stokes equations are adopted (Fan et al., 2007) to depict the flow field. LES is applied to treat the turbulence and the sub-grid scale (SGS) model of Smagorinsky (1963) is adopted.

The continuity and momentum equations for the unsteady, incompressible and isothermal airflow field after the filtering are as follows (Pope, 2000):

Continuity

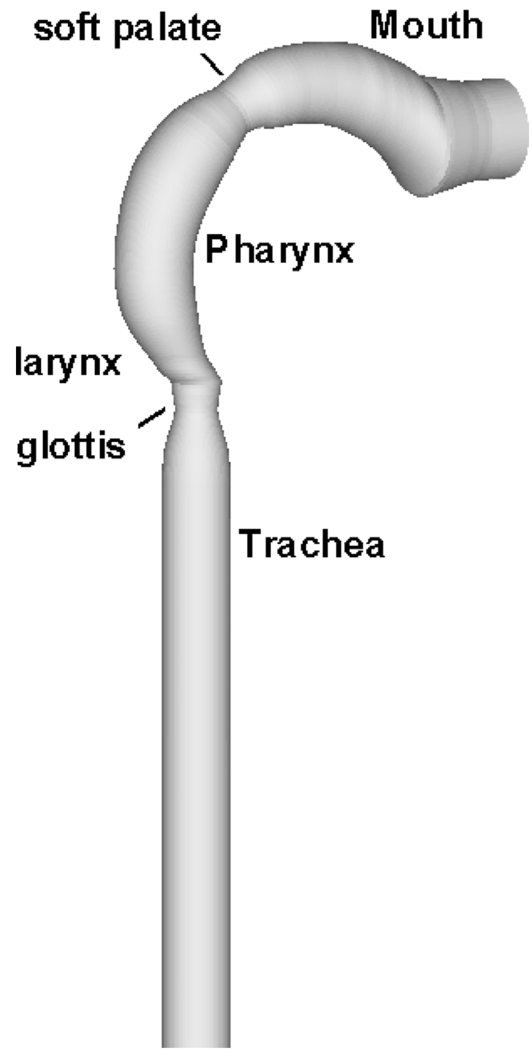

Fig. 1. Three-dimensional view of the circular idealized mouth-throat geometry. Reprinted from Kleinstreuer and Zhang (2003) with permission from © Elsevier.

$$\frac{\partial \overline{U}_j}{\partial x_j} = 0 \tag{1}$$

Momentum

$$\frac{\partial \overline{U}_i}{\partial t} = -\frac{\partial(\overline{U}_i\overline{U}_j)}{\partial x_j} - \frac{\partial \overline{p}}{\rho \partial x_i} + \frac{\partial}{\partial x_j}\left[\nu\left(\frac{\partial \overline{U}_i}{\partial x_j} + \frac{\partial \overline{U}_j}{\partial x_i}\right) - \tau_{\mathrm{ij}}^{\mathrm{r}}\right] \tag{2}$$

where U_i is the velocity component in i direction and the bar denotes filtered values, ρ is the gas density, ν the kinematic gas viscosity, p the static pressure, and $\tau_{\mathrm{ij}}^{\mathrm{r}}$ is the sub-grid scale stress tensor

$$\tau_{\mathrm{ij}}^{\mathrm{r}} = -2C_{\mathrm{s}}\Delta^2|\overline{S}|\overline{S}_{\mathrm{ij}}. \tag{3}$$

$\overline{S}_{\mathrm{ij}}$ is the strain rate tensor

$$\overline{S}_{\mathrm{ij}} = \frac{1}{2}\left(\frac{\partial \overline{U}_i}{\partial x_j} + \frac{\partial \overline{U}_j}{\partial x_i}\right). \tag{4}$$

Moreover,

$$|\overline{S}| = (2\,\overline{S}_{\mathrm{ij}}\overline{S}_{\mathrm{ij}})^{1/2}, \tag{5}$$

and $\Delta = (\Delta x \Delta y \Delta z)^{1/3}$ in Eq. (3) is the filter width. $C_{\mathrm{s}} = 0.165$ is the Smagorinsky constant (Lilly, 1967). In these equations, $i, j = 1, 2, 3$, and the Einstein summation convention is used.