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Three-dimensional unsteady large eddy simulation of the vortex structures and the mono-disperse particle dispersion in the idealized human upper respiratory system

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ABSTRACT

The present study concerns the three-dimensional unsteady large eddy simulation (LES) in an idealized human mouth-throat under the different inspiration flow rates of 15, 30 and 60 L/min. Three-dimensional vortices are observed in both the instantaneous and in the mean flow field in the mouth cavity, pharynx, larynx and trachea as well as in the recirculation zone of the pharynx. In the steady flow field it is found that the barrier caused by the tongue may induce hairpin vortices whereas the barrier glottis may cause horseshoe vortices. With the increase of the inspiration flow rate, the distance between the legs of the hairpin vortices in the mouth cavity decreases, and the length scale of the vortex in the trachea decreases with increasing inspiration flow rate. In the unsteady flow field, the counter-rotating vortices in the pharynx and trachea disappear at the highest inspiration flow rate, but the counter-rotating vortices can still be observed at the lowest inspiration flow rate. The vortex in the unsteady flow field is much more complex compared to the steady situation, and more vortices with smaller length scales are observed in the trachea for the increased flow rate. Lagrangian particle tracking is introduced into the model to investigate the process of particle drug delivery for medical treatment of the human airway. It is found that the mono-disperse particles may follow totally different trajectories depending on their initial release positions and the inspiration flow rates as well as on their size. The particles may follow very complex recirculating movements within the recirculation zone, and they may show a swinging, transverse or helical motion due to the vortex of the gas flow. This may also affect the deposition characteristics of the injected particles.

1. Introduction

Millions of people all over the world are burdened with respiratory diseases. A popular treatment of these diseases is the aerosol drug delivery via inhalers because of its advantage of rapid response, minimal systemic adverse effects and small doses. The human upper respiratory system is the first barrier for particles entering into the human body through breathing, and substantive drugs are filtered during the passage through the upper airway (Zhang, Kleinstreuer, & Kim, 2002). Thus, many investigations concern the properties of the flow field as well as the particle transport and deposition in the oral airway in order to improve the efficiency of the aerosol drug delivery.

During past decades, the numerical simulations have turned from solving the Reynolds averaged Navier-Stokes (RANS) equations

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to large eddy simulation (LES) in the upper respiratory system (Gemci, Ponyavin, Chen, Chen, & Collins, 2008; Matida, Ilie, & Finlay, 2008; Mylavarapu et al., 2009) because of the transitional character of the turbulence, and in this situation, the LES is superior to RANS modeling. In LES, a filter function separates the large and small length scales of turbulence, resolving the large scales, whereas the variables operating on the small scales are closed using a sub-grid scale model. Thus, its ability to predict the vortex structure of the flow field is better compared to RANS. Considerable research has been performed to investigate the properties of vortices in the upper human respiratory air stream. Vortices exist in the oral airway, in particular, they induce secondary streamlines at different cross-sections (Cui & Gutheil, 2011; Fan, Jin, Zeng, & Cen, 2007; Jayaraju, Brouns, Verbanck, & Lacor, 2007; Zhang et al., 2002). Recently, more attention has been paid to three-dimensional vortices. For instance, Pollard, Ball, & Uddin (2008a) show a vortex in the oral airway and the disorder flow structure in an extra-thoracic airway (ETA) built by Stapleton, Guentsch, Hoskinson, and Finlay (2000). In the same ETA, Pollard, Ball, & Uddin (2008b) exhibit distinct three-dimensional structures in the oro-pharynx region as well as repeated vortex structures in the trachea, but a detailed analysis of the vortex structure is not provided. Lin, Tawhai, McLennan, and Hoffman (2007) also demonstrate the existence of three-dimensional vortex structures in a intra-thoracic airway model, and they found these vortex structures to resemble those in an open cavity. Lin et al. (2007) studied the airflow in the upper respiratory system in a three-dimensional flow field, however, they did not introduce particles. They focused on the interaction of the airflow field and the laryngeal jet. Characteristics of the averaged flow field were compared at inspiration flow rates of 15, 30 and 60 L/min using RANS coupled with the low-Reynolds number (LRN) κ - ω model (Kleinstreuer & Zhang, 2003). However it is very important to focus on the vortex structures in the unsteady flow field with respect to their effect on the particle transport in the upper human respiratory system, and it is beneficial to address the vortex properties at different inspiration flow rates.

Moreover, the particle transport and deposition in the human upper airway was studied broadly. Zhang et al. (2002) demonstrated that particle trajectories are influenced by the recirculation zone of the air, and the fate of particles is related to their initial release position, but the details of these particle trajectories were not addressed in particular in the trachea, where the turbulence is predominant. The influence of the turbulent dispersion on the particle deposition is addressed by Fan et al. (2007) and Longest, Hindle, and Choudhuri (2009). Fan et al. (2007) found that the turbulence may influence the particle deposition because the particles not only deposit on the impact side but also at the lateral sides. Longest et al. (2009) observed that the droplet exhibits a recirculating motion in the vortical flow region, but no comparison of the particles transport is provided at different inspiration flow rates. Sun, Li, Xu, Zhao, and Tan (2014) investigated the vortex in a mouth-throat model at lower inspiration rates and they discuss the flow separation in the pharynx, but they did not compare the vortex dynamics and evolution at high inspiration flow rates. Three-dimensional vortex structures were identified by Banko, Coletti, Schiavazzi, Elkins, and Eaton (2015) in the oropharynx and the larynx of a three-dimensional anatomic model, and the flow field was studied experimentally in the upper and central human airways. Vortices were displayed in the mean flow field, but no three-dimensional vortex was shown in the airway for the unsteady flow. Moreover, the inspiration flow rate was not varied.

Concerning the LES modeling of the air flow in the upper human respiratory system, Agnihotri, Ghorbaniasl, Verbanck, and Lacor (2014) simulated the particle deposition using the multiple LES frozen field method. The methodology allows the decoupling of the particle simulation from the LES simulation, resulting in important savings of computational time, if different particle sizes are to be considered. A systematic procedure is presented for determining an optimal set with several instantaneous LES frozen fields. The numerical results show good agreement with experimental data and save computational time compared to the full LES simulation. They analyzed the deposition efficiency in different regions of the human oral airway. The comparison of the results of the Rotational-based Smagorinsky model (RoSM), which preserves the decay of the high wave number components, and those of the dynamic Smagorinsky model (DSM), shows nearly the same particle deposition efficiency. Similarly, Ghorbaniasl, Agnihotri, and Lacor (2013) found that the RoSM and the DSM subgrid scale models predict analogous flow field patterns in the human upper respiratory tract. The comparison of the DSM model with a $k - \omega$ sub-grid model also does not show significant difference with respect to the vortical flow field (Cui & Gutheil, 2011).

There are also some studies available that concern different mouth-throat geometries. Nicolaou and Zaki (2013) numerically studied the effect of mouth-throat geometry on the flow field and particle deposition efficiency in the mouth-throat cavity by analyzing four different MRI-based geometries. They performed direct numerical simulations (DNS) in order to obtain the transitional and turbulent flow fields. They conclude that particle deposition depends on the Reynolds number, which is directly affected by geometric factors. Furthermore, their results depict small recirculation and large separation regions in the larynx and trachea, respectively. Many studies have shown the pharyngeal jet and recirculation zones which develop right after the mouth due to the complexity of the geometry (Krause et al., 2013; Nicolaou & Zaki, 2013). Krause et al. (2013) numerically investigated the deposition of nanoparticles in the extrathoracic region by using the software platform OpenFOAM. They found that the k-ω SST turbulence model is suitable to illustrate the separation and recirculation regions in the pharynx and the larynx, and they report that their model overestimates the maximum values of the laryngeal jet velocity and the turbulent kinetic energy.

The idealized mouth-throat configuration of Kleinstreuer and Zhang (2003) is very popular and has been used in previous studies, but so far, no three-dimensional vortices have been discussed in this geometry. Therefore, in the present paper, the vortices in the idealized oral airway are presented and discussed under both steady and unsteady flow conditions and for different inspiration flow rates of 15, 30 and 60 L/min. The properties of the vortices will be analyzed in detail, and their effect on the particle motion will be studied.

2. Mathematical model

This section provides the numerical configuration, the governing equations as well as the numerical solution procedure.