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Numerical investigation of airflow in an idealised human extra-thoracic airway: a comparison study

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Abstract

Large eddy simulation (LES) technique is employed to numerically investigate the airflow through an idealised human extra-thoracic airway under different breathing conditions, 10 l/min, 30 l/min, and 120 l/min. The computational results are compared with single and cross hot-wire measurements, and with time-averaged flow field computed by standard $k-\omega$ and $k-\omega$ -SST Reynolds averaged Navier-Stokes (RANS) models and the Lattice-Boltzmann method (LBM). The LES results are also compared to root-mean-square (RMS) flow field computed by the Reynolds stress model (RSM) and LBM. LES generally gives better prediction of the time-averaged flow field than RANS models and LBM. LES also provides better estimation of the RMS flow field than both the RSM and the LBM.

Keywords

LES; hot-wire; RANS; LBM; RSM

1. Introduction

The airflow plays an important role in sleep-disordered breathing and inhalation of pharmaceuticals. Obstructive sleep apnea (OSA) is reported to affect approximately 4% of the United States population (Young et al 1993). It is now recognized to be an important health issue in western countries as well as in Hong Kong (Ip et al 2001). OSA is a disorder in which complete or partial obstruction of the upper airway during sleep (Victor 1999). When OSA occurs, it typically interrupts the patient sleeping (Huang 2007). In another application, inhaled pharmaceuticals are widely used for treatment of lung diseases, such as asthma, cystic fibrosis and chronic obstructive pulmonary disease. However, drug delivery rates to the alveolar regions of the lung are far from optimal. Typically 80–95% of an inhaled aerosol dose is deposited in extra-thoracic airway (ETA) (Gonda 1992). A better understanding of the unsteady flow field inside the airway, will allow us to learn more about the pathology of OSA and to achieve targeted drug delivery to the lungs.

Both hot-wire and particle image velocimetry (PIV) can be used to obtain unsteady velocity measurements and related properties in fluids. However, both of them have their own limitations (Johnstone 2003; Ball et al 2008). The experimental results from hot-wire are typically unreliable in regions with recirculation and secondary flow motion. PIV measurements are sometimes affected by optical access and seeding techniques.

An alternative approach to study flow is Computational Fluid Dynamics (CFD). With the fast development in computer technology and numerical methods during the past few decades, CFD has now become a standard approach to predict flows in large range of applications, including the non-linear transitional/turbulent airflow (Ball 2005; Jayaraju et al 2008; Kleinstreuer and Zhang 2009; Lee et al 2010; Mihaescu et al 2010). Turbulence is believed to be a typical feature of the flow in human airway. There are three main approaches to predicting the turbulent flow. Direct Numerical Simulation (DNS) involves numerical integration of the Navier-Stokes equations on a grid fine enough to resolve all the scales of motion from the airway geometry to the viscous dissipation scale. However, the involved computational costs make this approach prohibitive with current and near future computational resources. The RANS method involves ensemble averaging the Navier-Stokes equations over all length scales of the flow and only predicts the time-averaged flow. Mean flow predictions are much easier to perform than DNS and much more computationally affordable. However, they are sensitive to the geometry and flow conditions and may be inaccurate for separated turbulent flows. LES involves the direct computation of a large range of scales. Only the effects of the small scales on the large scales are modeled using a subgrid-scale model. The small scales are assumed to be universal in their behavior. LES can provide a better prediction for separated flows that feature high levels of unsteadiness. LES requires a sufficiently fine grid resolution and is more expensive than RANS but much more affordable than DNS. RANS has been widely utilized to investigate air-flows because of its low cost (Ball 2005; Ito et al 2011; Xu et al 2006). Recently, several groups have considered LES as an alternative approach for modeling airflows in human respiratory systems (Jayaraju et al 2008; Kleinstreuer and Zhang 2009; Lee et al 2010; Mihaescu et al 2010; Mylavarapu et al 2009; Zhao et al 2013).

Significant effort has been directed toward numerical modeling of airflows in human airway. However, accurate prediction of the flow in the ETA has not been achieved. It is expected that numerical predictions of particle deposition can be accurate only after singlephase CFD models are verified. Numerical studies have been performed to assess the capacity of RANS models to predict transitional flows. The RANS models are able to provide a qualitatively acceptable solution of the time-averaged airflow. However, it is very difficult for the RANS models to predict a quantitatively acceptable solution even for a simplified geometry and time-averaged flow field (Ball et al 2008). It seems even more difficult to predict flow fluctuations using RANS models. No report on turbulent stress prediction using RANS models in the idealised human airway was found (Ball et al 2008). Instead, LBM was applied to investigate the flow structures (Ball 2005). LBM is a novel class of CFD methods of fluid simulation. The discrete Boltzmann equation is solved instead of Navier-Stokes equations to simulate the flow of a Newtonian fluids with collision models. By simulating streaming and collision processes across a limited number of particles, the intrinsic particle interactions evince a microcosm of viscous flow behavior applicable across the greater mass. Some better agreement in the time-averaged flow field has been achieved using LBM than that using RANS models in FLUENT. However, the prediction of the flow fluctuations using LBM is still poor.

In this study, a static airway model is considered to avoid the effects of boundary movement on the flow. Employing the LES methodology, a detailed analysis of the velocity field is presented and compared with hotwire measurements, RANS computations, and LBM simulations.

2. Methods

The ETA is comprised of oral and nasal cavities, the pharynx, the larynx, and the trachea. As shown in Fig. 1, the idealised ETA presents a variety of cross-sectional shapes and

diameters. The diameter of the inlet tube is 19 mm and the diameter of the outlet is 16 mm. The length of the inlet tube is 50 mm and the length of the outlet tube is 62 mm. The total volume of this idealised model is about $8.83 \times 10^{-5} \text{ m}^3$. Flow rates of 10, 15, 30, 45, 60, 90 and 120 liters per minute for hot-wire measurements and 15, 30, and 60 liters per minute for flow visualization measurements are considered in the experiments (Johnstone 2003). The hot-wire measurements are accurate in regions where the flow is predominantly unidirectional. Their accuracy is diminished in areas of recirculation and reversed flow. These flow rates encompass a wide range of respiratory patterns, from normal tidal breathing to the rapid inhalation typically encountered during the use of pharmaceutical aerosol inhalation devices. The flow can range from laminar to turbulent. For the flow rates considered, the local Reynolds number, based on local mean diameter and local bulk velocity (Ball et al 2008), ranges from approximately 480 to over 12,000. Therefore, in order to accurately predict the flow, turbulence has to be resolved.

With the geometry data obtained from Prof. A. Pollard (Queen's University, Canada) in STereoLithography (STL) format by permission, TGRID (Ansys Inc.) is applied to generate the volume mesh for numerical simulation. The total number of the cells plays an important role in the computational cost. In order to decrease this number, a hexcore with boundary layers scheme is employed. One buffer layer and one peel layer are applied to the hexcore. The wall-bound control volume size is $y^+ = O(1)$ for all the flow rates, which is sufficiently small to capture wall effects. The first element layer thickness is 0.01 mm. The maximum $y^+ \approx 0.3$ was found at the inner side of station 6 in the 30 l/min case.

Unsteady LES is employed to investigate the air-flow in this study. This solver has been validated in previous studies (Mihaescu et al 2008; Mylavarapu et al 2009). Second order finite volume schemes are employed to discretize the flow governing equations on the computational domain. The time integration is performed using an implicit second order discretization scheme. The semi-implicit method for pressure-linked equation (SIMPLE) algorithm is applied to solve the coupling between the pressure field and velocity field (Patankar and Spalding 1972). The Smagorinsky-Lilly sub-grid scale model is employed as the subgrid-scale model in this study (Lilly 1966). The incompressible flow solver is employed for a complete characterization of the flow field. No-slip boundary conditions for velocity are set at the solid boundaries of the computational domain. Uniform velocity with 1% turbulent intensity is imposed at the inlet. At the outlet, the pressure outlet boundary condition is applied. A converged solution based on a steady state RANS solution with standard $k-\omega$ -SST turbulence model is used to initialize the LES simulations. The time step used in LES depends on the inlet flow rate Q . For example, when $Q = 30$ l/min, the time step is chosen to be $\Delta t = 1.0 \times 10^{-4}$ s. The mean flow quantities are statistically averaged over a period of 20,000 time-steps. The size of the grids is about 2.24×10^6 control volumes. It took nearly half a day to perform a steady state RANS $k-\omega$ -SST simulation on a four-core Intel Core Duo E8400 system and four weeks to complete an LES simulation on an eight-core Intel-Xeon x5650 system for the 30 l/min case.

3. Results and discussion

The boundary conditions play an important role in the flow simulation. In the experiments, a nozzle was added to the inlet of the model to decrease inlet losses and dampen out any external instabilities (Johnstone 2003). The use of a nozzle ensures virtually uniform inlet conditions at all flow rates, producing nearly plug flow (i.e. "top hat") inlet velocity profiles. Tests (Heenan et al 2003) show no effect of varying inlet condition on the mean flow field in steady RANS simulations. However, the steady RANS technique cannot accurately describe unsteady flow fields involving flow separation and adverse pressure gradients typical to the present geometry. In the past few decades, LES has become the major computational tool

for studying such unsteady turbulent flows. The specified turbulent intensity at the inlet plays an important role in calculating the fluctuations in the flow using LES.

The outflow condition is more appropriate where the exit flow is close to a fully developed condition, as it assumes a zero streamwise gradient for all flow variables except pressure. However, occasionally, reverse flow is found at the outlet during simulation. The use of a pressure outlet boundary condition often results in a better rate of convergence when backflow occurs during iteration. Therefore, as mentioned above, the pressure outlet boundary conditions have been considered here instead of the outflow condition as in the RANS simulations by Ball et al (2008).

Fig. 1 shows that the flow is nearly symmetric relative to the mid-sagittal plane because of the symmetry in the geometry. The uniform flow from the tube inlet becomes a free jet flow in the oral cavity and a recirculation zone develops. A second jet flow occurs at the transition of oral cavity and oropharynx, and another recirculation zone develops. As the airflow passes the epiglottis, because of the constriction in the larynx, a much stronger flow jet develops at the outer side (posterior) of larynx and attaches to the inner side (anterior) of the trachea, weakening as the flow reaches the outlet.

The pressure drop between inlet pressure and lowest pressure in the upper airway (Δp_{max}) may play an important role in the OSA severity. At the distal oral cavity and in the larynx, the higher velocities would indicate lower static pressures according to Bernoulli's theory. OSA typically occurs in the upper airway. Therefore, the distal oral cavity region needs more attention. The results in this study are similar to that in the computational research in a patient-specific airway after mandibular advancement splints (Zhao et al 2013). In fact, people with obstructive sleep apnea tend to sleep with their mouths open. The resulting Δp_{max} becomes lower resulting in a reduced airway susceptibility to collapse.

Local coordinate systems are defined corresponding to each of the measurement stations 1 to 7, as shown in Fig. 1, in order to simplify the interpretation of the flow results. As seen in Fig. 2(a), y axis is normal to the wall, with $y = 0$ at the outer side of the model, which is the superior side for stations 1 to 3 or posterior side for stations 4 to 7. The positive x axis is the same as the bulk flow direction at the station. Following the right hand rule, z is defined perpendicular to the mid-sagittal plane. U and V are the mean velocity components in the x and y directions. In the figures, L_{local} is the length of the y axis to the opposite wall inside the model. The subscript "rms" means root-mean-square (RMS). For a scalar ϕ , the RMS (ϕ_{rms}) is computed by employing its time-averaged mean $\bar{\phi}$

$$\phi_{rms} = \lim_{T \rightarrow \infty} \sqrt{\frac{1}{T} \int_0^T (\phi - \bar{\phi})^2 dt} \quad (1)$$

where T represents the time.

3.1 Station 1

As seen in Fig. 1, station 1 is very close to the location where the tube inlet meets the oral cavity. The jet flow is in the core region and is still circular, as shown in Fig. 2(d) for $Q = 10$ l/min. The recirculation zone develops around the core jet. The cross and single hot-wire measurements give nearly the same time-averaged streamwise velocity, exhibiting "top hat" profiles. The time averaged velocity components from the LES simulation, from the LBM simulation (Ball 2005) and from the standard $k-\omega$ and $k-\omega$ -SST RANS models are compared against the measurements. The standard $k-\omega$ model is a two equation model and includes two extra transport equations, turbulent kinetic energy k and specific dissipation ω , to

represent the turbulent properties of the flow. The $k-\omega$ -SST turbulence model employs a $k-\omega$ formulation in the inner parts of the boundary layer, thus rendering the model directly usable all the way down to the wall through the viscous sub-layer. Hence the $k-\omega$ -SST model can be used as a Low-Re turbulence model without any extra damping functions. The SST formulation also switches to a $k-\varepsilon$ behavior in the free-stream and thereby avoids the standard $k-\omega$ problem that the model is too sensitive to the inlet free-stream turbulence properties. The $k-\omega$ -SST model often has some advantage when used to predict adverse pressure gradients and separating flow (Menter 1994).

All computational results yield very good prediction in the core region. However, the hot-wire measurements near the wall are no longer reliable because of the recirculation as seen in Fig. 2(a). The difference between the measurements and the computations in the RMS streamwise velocity is significant. The magnitude of the fluctuation in the center is almost uniform while two peaks appear in the shear layers at both sides of the jet. The LES qualitatively captures both peaks while the LBM results are very different from the measurements. The difference between the LES and the LBM could result from different inlet turbulent intensity boundary conditions. Based on the RMS velocity components shown in Fig. 2 (c) and (f), it is reasonable to assume that the turbulent intensity at the inlet is around 1%, instead of 5% used in the RANS computations (Heenan et al 2003). In the transverse direction, LES results are much closer to the measurements than the LBM results. The LBM computation over-estimated the time averaged lateral velocity while under-estimating the RMS lateral velocity. It is interesting to note that the RANS models give more accurate estimation on the time-averaged transverse velocity than the LBM. For instance, at $y/L_{\text{local}} = 0.5$, the LES and RANS results are about 30% larger than the cross hot-wire measurement while the LBM simulation gives about 100% larger value than the time-averaged transverse velocity. As explained in the work by Ball (2005), this could be a scaling issue and the bulk velocity may not be the correct scaling factor for all velocity and turbulence results from the LBM simulation.

When the flow rate increases, the flow patterns are still very similar to the lower flow rate, as seen in Fig. 3. However, more complex flow patterns occur at the inner side of the model than the outer side. The LES computation still gives best prediction of the streamwise velocity in the core region. At the walls the difference becomes much larger because the hot-wire measurements are not accurate in the recirculation zone. Asymmetric double peaks appear in the RMS streamwise velocity in the measurements and similar asymmetric pattern is predicted by the LES results, representing the more complex flow at the inner side.

3.2 Station 3

Station 3 is located near the end of oral cavity. The flow becomes more uniform in the streamwise direction, as shown in Fig. 4(a). The hot-wire measurements show double peak in the time-averaged streamwise velocity profiles. The standard $k-\omega$ and $k-\omega$ -SST RANS models both fail to capture this phenomenon. Both the LBM and LES results qualitatively predict the streamwise velocity well while the LES results seems to be closer to the measurements. For instance, at $y/L_{\text{local}} = 0.6$, the LES result is about 15% lower than the hot-wire measurements while the LBM simulation gives about 30% lower value in the time-averaged streamwise velocity. The LES simulation also gives a better prediction of the RMS streamwise velocity than the LBM. All the computation results differ from the measurements in the time-averaged transverse velocity. Because the flow is predominantly in the streamwise direction, hot-wire measurements of transverse velocity component that deviates significantly from the streamwise direction are not accurate. However, the LES computation agrees well with the cross hot-wire measurements of the RMS transverse velocity.

As the flow rate increases, as seen in Fig. 5, the LES computation agree well with the hot-wire measurements in the time-averaged streamwise velocity while the RANS models fail again. Comparing the RMS stream-wise velocity, the LES results are now closer to the single hot-wire measurements.

3.3 Station 5

Station 5 is located inside the oropharynx, above the epiglottis, as shown in Fig. 6(a). The flow becomes very complex in this region. At the inner side (anterior), a recirculation zone appears because of the epiglottis. At the outer side (posterior), another recirculation zone appears due to the sudden expansion. The computation results qualitatively agree with the hot-wire measurements in time-averaged streamwise velocity. The computational results from the RSM (Ball 2005) are included in the comparison against the RMS streamwise velocity from the hot-wire measurements. The RSM provides very poor estimation, especially at the walls. As mentioned in the work by Ball (2005), the RSM prediction at stations 1 and 3 is even worse. The LES estimation in this study seems better than the LBM (Ball 2005). Double vortices appear in the cross section of station 5. It leads to difficulty in the hot-wire measurements due to the recirculation regions and the significant transverse velocity. As a result, both LBM and LES can only give a qualitative prediction in time-averaged and RMS transverse velocity and cannot be validated.

As flow rate increases, the flow patterns become somewhat different. The recirculation bubble attached to the epiglottis becomes larger, as shown in Fig. 7. At the top and bottom corner of the oropharynx, small recirculation zones appear at the outer side for $Q = 30$ l/min, however, the lower one disappears for $Q = 120$ l/min. LES predicts well the time-averaged streamwise velocity away from the outer side. At the outer side, the reverse flow leads to inaccurate measurements. In the RMS streamwise velocity, the LES shows qualitative agreement with the single hot-wire measurements.

3.4 Station 7

Station 7 is located inside the trachea as shown in Fig. 8. Similar to station 5, a big recirculation zone appears at the outer side so that the hot-wire measurements are not accurate. Both the LES computation in this study and the LBM results (Ball 2005) give qualitative good agreement with the hot-wire measurements in both the time-averaged and RMS streamwise velocity. The maximum in the RMS velocity appears in the shear layer of the flow. The RSM results (Ball 2005) differ from all models in the RMS streamwise velocity and give poor estimation at the wall.

4 Conclusions

In this study, LES is employed to numerically investigate the unsteady flow through an idealised human airway model. The computational results are compared with single and cross hot-wire measurements, and with standard $k-\omega$ and $k-\omega$ -SST RANS models, with RSM and LBM. In the work by Mihaescu et al (2008), the comparison was made between LES and RANS models, such as $k-\epsilon$ and standard $k-\omega$. That comparison was done without any experimental data while the present paper includes also comparison to a measure flow field. Also, the difference between LES and $k-\omega$ -SST RANS model was not discussed in the work by Mihaescu et al (2008).

The main conclusions are summarized as follows:

1. The hot-wire measurements are typically unreliable in regions with recirculation and secondary flow motion.

2. The boundary conditions play an important role in flow simulations. The inlet boundary conditions of the turbulent intensity typically alter the statistics of the velocity fluctuations near the inlet.
3. LES generally gives better prediction of the flow field than all the other numerical methods. The LES has great potential in predicting separated flows that feature high levels of unsteadiness.
4. The differences between the experimental and computational results are more significant with increasing Reynolds number, i.e., at higher flow rate.

In this work the airway model was rigid. In order to apply the computational technique discussed here to the study of airway collapse in OSA, the mechanical properties of the airway soft tissues must be considered using fluid-structure interaction. Also, to study aerosolized drug delivery (Jayaraju et al 2008), interaction between flow and particles should be modeled. Our current research extends this study to the application of LES to OSA and aerosolized drug delivery.

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Fig. 1.
(Color online) Time-averaged velocity magnitude contours on the mid-sagittal plane and the cross sections of the measurement stations, 30 l/min

Fig. 2.

(Color online) Station 1: (a) RMS velocity magnitude contours and streamlines of the time-averaged flow field on the mid-sagittal plane, (b) Time-averaged and (c) RMS streamwise velocity profiles, (d) Time-averaged velocity magnitude contours and streamlines in the cross section, (e) Time-averaged and (f) RMS lateral velocity profiles, 10 l/min

Fig. 3.

(Color online) Station 1: (a) RMS velocity magnitude contours and streamlines of the time-averaged flow field on the mid-sagittal plane, (b) Time-averaged and (c) RMS streamwise velocity profiles, 30 l/min; Station 1: (d) RMS velocity magnitude contours and streamlines in the time-averaged flow field on the mid-sagittal plane, (e) Time-averaged and (f) RMS streamwise velocity profiles, 120 l/min

Fig. 4. (Color online) Station 3: (a) RMS velocity magnitude contours and streamlines of the time-averaged flow field on the mid-sagittal plane, (b) Time-averaged and (c) RMS streamwise velocity profiles, (d) Time-averaged velocity magnitude contours and streamlines in the cross section, (e) Time-averaged and (f) RMS lateral velocity profiles, 10 l/min

Fig. 5.

(Color online) Station 3: (a) RMS velocity magnitude contours and streamlines of the time-averaged flow field on the mid-sagittal plane, (b) Time-averaged and (c) RMS streamwise velocity profiles, 30 l/min; (d) RMS velocity magnitude contours and streamlines in the time-averaged flow field on the mid-sagittal plane, (e) Time-averaged and (f) RMS streamwise velocity profiles, 120 l/min

Fig. 6.

(Color online) Station 5: (a) RMS velocity magnitude contours and streamlines of the time-averaged flow field on the mid-sagittal plane, (b) Time-averaged and (c) RMS streamwise velocity profiles, (d) Time-averaged velocity magnitude contours and streamlines in the cross section, (e) Time-averaged and (f) RMS lateral velocity profiles, 10 l/min

Fig. 7.

(Color online) Station 5: (a) RMS velocity magnitude contours and streamlines of the time-averaged flow field on the mid-sagittal plane, (b) Time-averaged and (c) RMS streamwise velocity profiles, 30 l/min; (d) RMS velocity magnitude contours and streamlines in the time-averaged flow field on the mid-sagittal plane, (e) Time-averaged and (f) RMS streamwise velocity profiles, 120 l/min

Fig. 8.

(Color online) Station 7: (a) RMS velocity magnitude contours and streamlines of the time-averaged flow field on the mid-sagittal plane, (b) Time-averaged and (c) RMS streamwise velocity profiles, 10 l/min; (d) RMS velocity magnitude contours and streamlines in the time-averaged flow field on the mid-sagittal plane, (e) Time-averaged and (f) RMS streamwise velocity profiles, 30 l/min