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Characteristics of the turbulent laryngeal jet and its effect on airflow in the human intra-thoracic airways

Ching-Long Lin^{a,b}, Merryn H. Tawhai^f, Geoffrey McLennan^{c,d,e}, and Eric A. Hoffman^{c,d,e}

^a Department of Mechanical and Industrial Engineering, The University of Iowa, Iowa City, Iowa 52242

^b IIHR-Hydroscience & Engineering, The University of Iowa, Iowa City, Iowa 52242

^c Biomedical Engineering, The University of Iowa, Iowa City, Iowa 52242

^d Medicine, The University of Iowa, Iowa City, Iowa 52242

^e Radiology, The University of Iowa, Iowa City, Iowa 52242

^f Bioengineering Institute, The University of Auckland, Auckland, NZ

Abstract

A computational fluid dynamics technique is applied to understand the relative importance of the upper and intra-thoracic airways and their role in determining central airflow patterns with particular attention paid to the importance of turbulence. The geometry of the human upper respiratory tract is derived from volumetric scans of a volunteer imaged via multidetector-row computed tomography. Geometry 1 consists of a mouth piece, the mouth, the oropharynx, the larynx, and the intra-thoracic airways of up to 6 generations. Geometry 2 comprises only the intra-thoracic airways. The results show that a curved sheet-like turbulent laryngeal jet is observed only in geometry 1 with turbulence intensity in the trachea varying from 10% to 20%, whereas the turbulence in geometry 2 is negligible. The presence of turbulence is found to increase the maximum localised wall shear stress by three folds. The proper orthogonal decomposition analysis reveals that the regions of high turbulence intensity are associated with Taylor-Görtler-like vortices. We conclude that turbulence induced by the laryngeal jet could significantly affect airway flow patterns as well as tracheal wall shear stress. Thus airflow modeling, particularly subject specific evaluations, should consider upper as well as intra-thoracic airway geometry.

Keywords

MDCT-based airway model; computational fluid dynamics; turbulence; laryngeal jet; ventilation; computed tomography

1. Introduction

Understanding the detail of flow in the pulmonary airways is prompted by two main areas of interest: particle transport, and the effect of airway abnormalities. The deposition of therapeutic or pollutant particles is dependent on the characteristics of the flow by which they are

Send correspondence to: Ching-Long Lin, Ph.D., Department of Mechanical and Industrial Engineering, The University of Iowa, Iowa City, IA 52242-1527, USA, 319-339-5673 (Voice), 319-339-5669 (Fax), ching-long-lin@uiowa.edu.

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transported. The flow is, in turn, dependent on the geometry of the airways and how ventilation is distributed to the peripheral tissue. An understanding of the structure-flow relationship is the first critical step in designing particulates to target specific sites in the lung, or for studying which populations are most susceptible to inhaled pollutants. Airway abnormalities serve as the pathophysiologic basis for many pulmonary diseases, including gross abnormalities such as idiopathic subglottic stenosis (Graham et al. 2000) or the stenosis that follows prolonged intubation and mechanical ventilation, and the more subtle changes associated with asthmatic airway remodeling. A change to upper or central airway geometry also potentially alters the location of the isothermal saturation boundary (the location where inspired air reaches body temperature and saturation), and will alter mechanical shear stress acting on the airway mucosa. If the nature of the flow is turbulent this may increase localised shear stress and will have a major effect on mixing and transport of particles.

With rapid advances in medical imaging, computer technologies, and computational techniques, computational fluid dynamics (CFD) is now becoming a viable tool for analysing airflow in the human respiratory tract. The complexity of the human tracheobronchial tree has restricted the majority of previous CFD studies to small regions of the airway tree, with the complex domain represented by idealised cylindrical branching geometries over a few generations (e.g. Comer et al., 2000, 2001a, 2001b; Nowak et al., 2003; Zhang and Kleinstreuer, 2002, 2004). An exception is van Ertbruggen et al (2005), who simulated flow and particle transport through a more extensive geometry, based on Horsfield's description of the airway tree (Horsfield et al. 1971) from the trachea up to generation 7. While this study presented a more extensive estimate of flow in the lung, it still relied on an idealised smooth representation of the airway geometry and ignored the effect of turbulence. Even with such severe limitations on the size and complexity of previous airway models, CFD simulation has been used in physiological studies of airflow. For example, in an attempt to understand particle deposition in the development of lung cancer (Balásházy et al., 2003), and in targeting delivery of therapeutic aerosols (Kleinstreuer and Zhang, 2003).

Most reported CFD analyses (including those previously cited) do not include the oropharyngeal and laryngeal regions. Zhang and Kleinstreuer (2004) studied airflow and nano-particle deposition in the oropharynx, the larynx and an airway tree of 4 generations, however their analysis used an idealised tubular geometry throughout the domain. Brouns et al. (2006) simulated flow in an idealised model based on magnetic resonance imaging (MRI) from the oropharynx to the end of the trachea, mainly to understand the influence of glottal aperture shape on airflow. They concluded that future models require more geometric detail than their smooth average geometry.

Airway CFD models that lack an oropharynx and larynx must instead specify a boundary condition at the tracheal 'inlet'. This boundary condition is often assumed to be a fixed/cyclic velocity or pressure (van Ertbruggen et al., 2005; Nowak et al., 2003). The flow is further assumed to be either laminar (van Ertbruggen et al., 2005; Nowak et al., 2003) or turbulent (Stapleton et al., 2000; Zhang and Kleinstreuer, 2004). The three approaches for simulation of turbulent flows are direct numerical simulation (DNS), large-eddy simulation (LES), and Reynolds-Averaged Navier-Stokes (RANS) models. DNS is the most accurate technique and resolves turbulent eddies at all scales, but it is also the most computationally expensive, and is only suitable for low Reynolds (Re) turbulent flows (Pope, 2003). LES resolves large-scale energy-containing turbulent eddies and parameterizes small-scale unresolved eddies. RANS does not resolve any turbulent eddy structures and uses a turbulence model to predict the dynamics of these eddies. The popular RANS turbulence models are $k-\epsilon$ and $k-\omega$ models, which are expected to be inaccurate for many non-equilibrium turbulent flows (Pope, 2003; Wilcox, 1994). Previous studies have concluded that RANS does not adequately capture the viscous

effects at lower Re (Heenan et. al., 2003) and that the k- ϵ model is not accurate for particle tracking in the range of Re found in the oropharynx (Stapleton et al., 2000).

Two major issues have not been addressed to date in CFD studies of airway flow: 1) a realistic geometry that reflects the detail of the *in vivo* human airway has not been investigated, and 2) the characteristics of the turbulent laryngeal jet and its effect on airflow in the intra-thoracic airways remains unclear. The current study presents construction of a realistic geometry of the upper respiratory tract from MDCT images acquired from a single human subject. The geometry includes a mouth piece, the mouth, the oropharynx, the larynx, and the airways of ~6 generations. The dependence of airflow in the intra-thoracic airways on the complex oropharyngeal and laryngeal geometry is studied by comparing two cases: the first uses the complete geometry, and the second uses only the intra-thoracic airway tree geometry. The relationship between turbulent structures and airway anatomy is of particular interest as we move to better understand patterns of inhaled drug delivery, effects of air pollution on individuals, effects of disorders which alter airway geometries on patterns of gas flow to the lung and more. It is possible, for instance, that in some subjects a particular airway geometry leads to a pattern of airway turbulence induced by a laryngeal jet which might cause enough shear stress on the tracheal epithelium to disrupt mucosal healing processes. This could lead to fibrosis, particularly if the mucosa has already been primarily injured by an infection or mechanical pressure from an inflated endotracheal tube balloon. An analogous situation has been reported in the development of vascular stenosis associated with abnormal blood flow (Doriot and Dorsaz, 2004; Prado et al., 2006). Hence, in this paper the turbulent structures in the supraglottis, the glottis, the subglottis and the main-stem bronchi are investigated and the localised wall shear stresses with or without the presence of turbulence are compared.

2. METHODS

2.1 MDCT Image Acquisition and Reconstruction

Imaging used in this study was acquired under a Bioengineering Research Partnership (NIH R01-HL-064368), and was approved by the University of Iowa Institutional Review Board. Data were derived from one normal human subject from the Human Lung Atlas, acquired at the Iowa Comprehensive Lung Imaging Center (I-Clic), The University of Iowa, by use of a Siemens Sensation 64 MDCT scanner. Scan parameters were: 120 kV, 100 mAs, pitch 1.2, slice width 0.6 mm, slice interval 0.6 mm. Images consisted of a spiral scan of the full lung and upper airway (to the roof of the soft pallet) with inflation level held at 95% vital capacity. Subjects were imaged supine. The human subject with a study identification of H-869 was a white, non-Hispanic 20 year old female, weight 62.1 kg, height 170.6 cm, and body mass index (BMI) 21.34. The subject was a non-smoker with FEV1 of 3.47 l/min (93.03%), forced vital capacity 3.45 l (80% predicted), TLC 6.22 liters (113% predicted) and diffusing capacity 28.6 ml/mmHg/min of CO (89%).

The MDCT images were processed using an in-house derived software package (VIDA/PASS) to segment the lungs, lobes and intra-thoracic as well as upper airways (Aykan et al., 2003; Guo et al., 2002; Hoffman et al., 1992; Palagyi et al., 2005; Tschiren et al., 2005a, 2005b). VIDA/PASS is based upon a combination of three-dimensional (3D) region growing and 2D mathematical morphology methods (Aykan et al., 2003). It has been demonstrated that the software can successfully extract airway trees from most clinical quality standard-dose MDCT data (Tschirren et al., 2005a).

The surface geometry segmented from MDCT images was exported to an STL (STereo-Lithography) file. The STL file was then imported into Magics® for smoothing rough edges and clipping off the trachea (or mouth) and the terminal airways to create inlet and outlet faces for specification of boundary conditions for numerical simulation. Fig. 1, A and B, display the

top and oblique views of the MDCT-based mouth-oropharynx-larynx-trachea structure. The mouth and teeth of the human subject are clearly resolved by the MDCT images. A mouth piece was used to provide precise lung volume control for the MDCT scanning. Fig. 1B shows the internal structure of the upper respiratory tract by splitting the geometry along the white line in Fig 1A.

Fig. 1, C and D, show the airway tree of the subject, with the major airway bronchial segments labeled using a modified version of the internationally accepted standard nomenclature. To allow description of airway segments between identified branch points, TriLUL, TriRUL, and TriLLB have been added to describe branch points in the origins of the left upper lobe (LUL), the right upper lobe (RUL), and the left lower lobe (LLL) respectively. The characteristics of the airway tree, in terms of average area, diameter, and length, are listed in table 1. The quantitative information is extracted from the MDCT images using the VIDA/PASS software. The oblique view of the airway tree is displayed in Fig. 1D to reveal the rings in the trachea and the left main-stem bronchus (LMB) and the airway branches located at the rear side of the lung. The trachea is counted as generation 0, and the current airway tree consists of up to 6 generations of branches.

2.2 Computational Methods

The governing equations for incompressible fluid flow are composed of the continuity equation and the Navier-Stokes equations. In tensor notation, they are

$$\frac{\partial u_j}{\partial x_j} = 0 \quad (1)$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\nu \frac{\partial u_i}{\partial x_j} \right) \quad (2)$$

where u_i , p , ρ , and ν are the velocity components in the i -direction, pressure, density, and kinematic viscosity, respectively. Here the Einstein summation is invoked so that the repeated index implies summation. The continuity equation, Eq. 1, is enforced by solving a pressure-Poisson equation. The air properties used for the study are a density of 1.2 kg/m^3 and a kinematic viscosity of $1.7 \times 10^{-5} \text{ m}^2/\text{s}$. Hereafter (x_1, x_2, x_3) and (x, y, z) are interchangeable, so are (u_1, u_2, u_3) and (u, v, w) . The second-order characteristic Galerkin fractional four-step method is applied to solve the coupled Eqs. 1 and 2 with the time step determined by the CFL condition. Details of the computational methods and several benchmark cases for accuracy of the scheme are reported in Lin et al. (2005).

Due to the low Re nature of the flow in the current study, DNS is used to simulate turbulence if it is present in the flow field. To estimate the numerical error that may be incurred by the mesh size, we present in Appendix A the results of model validation and subgrid-scale (SGS) estimation. The SGS eddies are referred to as the turbulent eddies that are too small to be resolved adequately with a given mesh.

2.3 Study Cases and Boundary Conditions

To study the dependence of airflow in the intra-thoracic airways on the oropharynx and larynx, two cases are considered. In case 1, the entire geometry comprising a mouth piece, the mouth, the oropharynx, the larynx, and the intra-thoracic airways, as shown in Fig. 2, A and B, is adopted for simulation. In case 2, only the intra-thoracic airway tree, as shown in Fig. 1, C and D, is used for simulation.

Boundary conditions for pressure or flow (or velocity) must be specified at each inlet and outlet of the two model cases. In case 1 inclusion of the mouth and oropharynx geometry substantially simplifies the boundary condition at the inlet of the mouthpiece and eliminates the need for approximation of the velocity at the tracheal opening. Thus a uniform pressure is imposed at the inlet of the mouthpiece (tracheal opening) for case 1 (case 2). At the outlets of the terminal branches for both cases, we assume uniform ventilation and specify uniform velocity. This allows the air to develop the velocity profiles at the mouthpiece and the trachea for cases 1 and 2, respectively. The current study aims to compare the two geometry cases, hence the most important criteria is that the boundary conditions in the two models are the same.

The magnitude of the velocity vectors on the outward normal faces of the terminal airways are set at 1.74 m/s, which corresponds to a volumetric flow rate of $\sim 3.2 \times 10^{-4} \text{ m}^3/\text{s}$ (320 ml/s) at the peak inspiratory phase through the mouth as well as the trachea. The flow is within the physiological range of normal human breathing. For the specified flow the mean speed through the trachea is $\sim 2 \text{ m/s}$, corresponding to $\text{Re} \sim 1,700$, which is computed based upon the mean speed of airflow in the trachea and the average diameter of the trachea (table 1).

2.4 3D Mesh and Data Acquisition

The STL files for the airway geometry described in section 2.1 are imported into Gambit® for mesh generation. The mesh for case 1 contains 1,390,808 nodes and 7,115,300 tetrahedral elements, whereas the mesh for case 2 has 454,165 nodes and 2,136,160 tetrahedral elements. Fig. 3A shows a snapshot of the fine surface mesh for case 1, and Fig. 3B displays the 3D interior mesh intersecting with a horizontal plane at $y = 0 \text{ m}$. The average grid distance near the tracheal wall in wall units, viz. normalized by ν/u_τ where u_τ is the friction velocity, is about 3.7. Because of the large mesh size and the requirement for time-accurate solutions, the simulations were run on the Tungsten super-cluster at the National Center for Supercomputing Applications (NCSA). The meshes for cases 1 and 2 were partitioned into 128 and 32 sub-domains and the computations were executed on 128 and 32 computer processors simultaneously. Each output file for case 1 (case 2) has a size of ~ 520 (~ 160) M bytes.

To estimate the time duration and interval for outputting files, two virtual point sensors are placed along the centerline of the trachea at $y = 0.04$ and 0 m (refer to Fig. 2 regarding these two locations with respect to the entire geometry) to record the time history of u , v , and w velocity components and p/ρ (note that density is a constant, therefore, p and p/ρ have the same frequencies). Fig. 4 plots the time variation of those quantities for case 1 at $y=0.04 \text{ m}$. It shows that case 1 is unsteady and turbulent. By the spectral analysis of these signals, the time periods of the peak fluctuating mode are found to be 0.0857, 0.16, 0.1143, and 0.0686 s for u , v , w , and p/ρ , respectively. The analysis of the data measured at $y=0 \text{ m}$ yields the time periods of 0.2182, 0.16, 2.4, and 0.0686 s for u , v , w , and p/ρ . Based on these periods, the time interval of 0.024 s selected for sampling data is adequate to ensure temporal resolution of pressure fluctuations (which has the smallest time period) through satisfaction of Nyquist sampling rate. The data are gathered over a time duration of 6 s, yielding 250 volume data sets for case 1. Here the volume data are referred to as the velocity and pressure fields of the air in the 3D airway geometry. The first 50 volumes of data are excluded in calculation of turbulence statistics to minimize the turbulence spin-up effect. The flow for case 2 is essentially laminar as is discussed later, however 100 volumes of data are still used for post-processing.

The mean of a physical quantity f is calculated by $\bar{f}(x_i) = \sum_{k=1}^{N_v} f(x_i, t_k) / N_v$, where the over-bar denotes a time average, t_k denotes the time of the k th volume data, and N_v is the number of volume data. The values of N_v for cases 1 and 2 are 200 and 100, respectively. For example, the mean values of velocities and pressure are represented by the horizontal solid lines in Fig. 4. The instantaneous turbulent fluctuation can then be computed by $f'(x_i, t_k) = f(x_i, t_k) - \bar{f}(x_i)$.

The turbulent kinetic energy (TKE) is defined as $\overline{(u'^2 + v'^2 + w'^2)}/2$, and the mean kinetic energy (MKE) is defined as $(\bar{u}^2 + \bar{v}^2 + \bar{w}^2)/2$. The turbulence intensity is defined as the ratio of the turbulent velocity fluctuation over the mean speed, calculated as $\sqrt{TKE/3MKE}$.

2.5 Proper Orthogonal Decomposition

To understand turbulent coherent spatial structures and their spectral signatures in a deterministic manner, the proper orthogonal decomposition (POD) technique is applied to the velocity fields. The POD was proposed by Holmes et al. (1996) for identification of coherent structures in turbulence. The notion behind the POD is to project an ensemble of scalar or vector fields onto candidate basis functions in time and space through optimality. The spatial orthonormal eigenmodes of the POD are called topos ψ_k , and the temporal orthonormal eigenmodes are called chronos ϕ_k . The decomposition based on a database of M snapshots of field data reads

$$s(x_i, t) = \sum_{k=1}^M \mu_k \phi_k(t) \psi_k(x_i) \quad (3)$$

where s represents scalar or vector fields and $\lambda_k = \mu_k^2$ are the eigenvalues of the decomposition (Pastur et al., 2005). The POD has been applied to study spectral signature and self-sustained oscillations in the flow over open cavities (Pastur et al., 2005; Rowley and Williams, 2006). The eigenmodes can be calculated by the method of snapshots (Holmes et al., 1996), which involves construction of the time-correlation matrix:

$$C(t, t') = \iiint_{\Omega} s(x_i, t) s(x_i, t') dx_i \quad (4)$$

where Ω denotes a volume and $s(x_i, t)$ are M instantaneous snapshots of scalar or velocity fields. In matrix form, these M snapshots of field data with each of them containing N computational nodes (or experimental pixels) can be stored in a data matrix A whose column entities are the nodal values of numerical data (or the pixels of experimental data) at a given snapshot. Therefore, the size of matrix A is $N \times M$ for a scalar field, and $3N \times M$ for a vector field. The time correlation matrix C is calculated by $C = A^t A$, where the superscript t denotes transpose of a matrix. The temporal eigenmodes, chronos, are obtained by applying a singular value decomposition to the matrix C and the corresponding eigenvalues of the decomposition are λ_k , representing the energy of the k th eigenmode. The spatial eigenmodes, topos, are then given by

$$\psi_k(x_i) = 1/\mu_k \int_{\Gamma} \phi_k(t) s(x_i, t) dt \quad (5)$$

where Γ denotes the time duration of these M snapshots of data. The eigenvalues are ordered from the largest ($k=1$) to the smallest values ($k=M$), and so are the associated eigenmodes. Thus, ψ_1 and ϕ_1 are the most energetic eigenmodes. For a more detailed description of the technique, please refer to Holmes et al. (1996) and Pastur et al. (2005). The POD analysis is applied to three zones of interest as marked in Fig. 2 and listed in table 2. Zone 1 is the region $0.04 \leq y \leq 0.10$ m including the laryngopharynx, the supraglottic space, and the glottis. Zone 2 is the region $-0.02 \leq y \leq 0.04$ m including the subglottic space and the trachea. Zone 3 consists of the first bifurcation ($y \leq -0.085$ m), and the LMB and RMB. The fluctuating velocity vector fields are used to extract 3D spatial structures. The sizes of data matrix A $3N \times M$ for zones 1, 2, and 3 are $(N:M)=(287,731:200)$, $(101,442:200)$, and $(101,244:200)$, respectively.

3. RESULTS

3.1 Characteristics of Mean Velocity Structures

Fig. 5, *A* and *B*, display the 3D isosurface of mean speed at 2 m/s for case 1. A high-speed laryngeal jet is formed as the flow passes through the glottis. It then jets into the trachea at an angle of $\sim 20^\circ$ with respect to the centerline of the trachea. Flow separation and recirculation are found at the location marked by the arrow in Fig. 5*B*. The flow then impacts on the back of the tracheal wall and creates a sheet-like high-speed zone curved against the wall as the jet moves deeper down the trachea. In contrast, the results for case 2 shown in Fig. 5, *C* and *D*, exhibit different features. In particular, the jet in the trachea has a maximum along the centerline of the trachea, similar to a 3D parabola, as seen from the front and side views. Also noted is the difference between the structures near the first bifurcation. Fig. 5*C* indicates that, perhaps due to the concentrated high-speed parabola in case 2, the stagnation low-speed zone is smaller in size than that of case 1. Subsequently the air flowing to both the left and the right lungs for case 2 exhibits a more concentrated core of high velocity than that of case 1.

To further compare the two cases, the velocity vectors and isosurface of speed in the three cross sections marked by S.1, S.2 and S.3 in Fig. 5 are displayed in Fig. 6. Rotational motion is observed in the trachea of case 1 (Fig. 6*A*), but is absent in case 2 (Fig. 6*D*). The contours of mean speed for case 1 further confirms the formation of a sheet-like high-speed zone, which is especially evident on the left-hand side of the figure, and the maximum velocity is biased toward the rear wall of the trachea. The left main-stem bronchus (LMB) in Fig. 6, *B* and *E* shows maximum speed biased toward the inner wall of the bifurcation in both case 1 and 2, however the high-speed zone for case 2 is much more concentrated (Fig. 6*E*) and creates more defined counter-rotating vortices than case 1 (Fig. 6*B*). In the right main-stem bronchus (RMB) neither case clearly exhibits counter-rotating vortices due to the oval-like cross section and the larger cross-sectional area of the RMB relative to the LMB (see table 1). In addition, after splitting the flow at the end of the RMB the flow is not biased toward the inner wall of the bifurcation. This is because the child branch TriRUL is almost perpendicular to the parent branch RMB as compared with the other daughter branch BronInt (intermediate bronchus) whose orientation is almost parallel to that of RMB. Thus, the inertia effect does not favor flow biasing toward the inner wall of the branch BronInt.

3.2 Turbulence Statistics

To gain insights into the turbulent characteristics of lung airflow, we analyse MKE, TKE, and turbulence intensity. If the flow is laminar, TKE is zero. In the region with a large TKE, the flow is more turbulent, likely resulting in effective mixing of gases and particulate matters and high wall shear stresses. Fig. 7, *A*, *B*, and *C* (*D*, *E*, and *F*), display the contours of MKE, TKE, and turbulence intensity for case 1 (case 2) in a vertical plane at $z = 0$ m (see Fig. 2*B*). For case 1, the MKE contours consistently reveal the sheet-like feature of the mean flow, with two local maxima located near the side wall of the trachea except in the vicinity of the vocal cords and the first bifurcation. After the first bifurcation, a high MKE is found in the LMB of case 1. In contrast, for case 2 a velocity parabola is developed along the trachea with the local maximum found along the centerline as shown in Fig. 7*D*. Furthermore, the MKE of the air flowing into the RMB is about the same as that of the LMB for case 2.

The TKE contours for case 1 in Fig. 7*B* indicate that the jet near the top of the trachea exhibits three regions of high turbulence strength: the core of the jet and two thin narrow line-like zones near the wall. The latter results from a plane cutting through a sheet-like structure discussed above. The TKE value in the lower part of the trachea drops by a factor of ~ 2 and the TKE values in the LMB (generation 1), RMB (generation 1), and LLB (generation 2) and BronInt (generation 2) are further reduced to various degrees. The TriLUL and TriRUL (both generation

2), which branch off from the LMB and RMB at an angle of $\sim 90^\circ$, contain less TKE, suggesting that these two branches and their associated child branches (and beyond) are not notably affected by the laryngeal jet.

For case 2, Fig. 7E shows that TKE is 400 times weaker than case 1 (note that the contour levels for Fig. 7, B and E, are different). The negligible, but non-zero, TKE along the tracheal centerline may be attributable to the uniform pressure imposed at the tracheal opening. Thus, the flow for case 2 can be treated as quasi-steady laminar flow.

Fig. 7C displays the contours of turbulence intensity for case 1. A contour level greater than 20% is found in the subglottic space, having a spatial distribution resembling that of TKE. In some lower and central parts of the trachea, the intensity decreases to $\sim 10\%$. Several regions of high turbulence intensity coincide with stagnation and separation regions, where mean velocities are small. The intensity in the LMB and RMB varies from 5% to 20%. Fig. 7C also suggests that the branch LLB6 (see Fig. 1C) has a high intensity at its entrance and along the wall. By inspecting Fig. 5A, the high-speed zone leaving the LMB enters the LLB6 to form a narrow high-speed zone. From Fig. 7C, this narrow zone is unsteady and might swing between walls, resulting in high turbulence intensity near the wall. For case 2, the turbulence intensity is essentially zero, as shown by its contours in Fig. 7F.

Before closing this subsection, we shall examine the relationship of the laryngeal jet to the oropharynx geometrical structure. Fig. 8A shows the contours of TKE in a vertical plane of $x = 0$ m. There are strong turbulent motions deep in the mouth. As the air passes the epiglottis (see Fig. 1B), a high TKE reappears and reaches a local maximum at the bifurcation between the larynx and the esophagus. The cross section at station B in Fig. 8A shows that the strong turbulence activity is found at the inner wall of the bifurcation. A comparison with the isosurface of the mean speed in Fig. 5B indicates that this bifurcation is at the location where a strong laryngeal jet begins to take shape.

Below the vocal cords in the larynx at station C the TKE contours exhibit a ring-like distribution as illustrated in Fig. 8C. The geometry between C and D resembles a backward facing step and a curved pipe, where flow recirculation is formed. A high TKE is found at the interface between the cavity flow and the free stream velocity. A cross-sectional view of the TKE contours at station D is displayed in Fig. 8D, which shows a mixed feature with a ring-like structure as noted in Fig. 8C. At station E in the trachea, Fig. 8A shows a second high TKE strip is formed at the front end of the trachea. From the cross-sectional view of Fig. 8E, the strip corresponds to a local maximum, while the rest of the TKE contours resemble that of Fig. 8D. It is speculated that the strip originates from the ring-like structure observed in Fig. 8, C and D, and is formed when the ring breaks up due to the converging cross-sectional area. The presence of strong turbulence between D and E results in a localised wall shear stress of up to $\sim 0.3 \text{ N/m}^2$, which is about 3 times stronger than that of case 2 in the absence of turbulence.

3.3 POD Analysis

To understand the relationship between local TKE maxima and airway anatomy, we apply the POD technique to extract turbulent coherent structures. A convergence test of the POD solution is first performed on zone 2 (see Fig. 2 and the region between planes C and E in Fig. 8) where the maximum turbulence intensity is located by gradually increasing the number of snapshots of the velocity field data M . The convergence error is measured and quantified by the normalized L1 norm η between the most energetic eigenmode solutions ($k = 1$) obtained from M and $M-1$ snapshots of data.

$$\eta = \left(\iiint_{\Omega} \|\psi_1^M - \psi_1^{M-1}\| dx_i \right) / \iiint_{\Omega} |\psi_1^{200}| dx_i \quad (6)$$

The test shows that the convergence errors η are 0.125, 0.071, 0.060, 0.032, and 0.016 at $M=20, 50, 100, 150$, and 200, confirming the convergence of the POD solution. The TKE

fractions of the first and second eigenmodes computed from $\lambda_i / \sum_{k=1}^M \lambda_k$ with $i=1$ and 2 for the three zones are given in table 2. The TKE fractions of the first eigenmodes in zones 2 and 3 are ~15% as compared with ~7% in zone 1. The TKE fraction in these zones drops to ~3% at the 10th eigenmode and to less than 1% at the 50th eigenmode. The characteristic frequencies and periods of these spatial eigenmodes as listed in table 2 are obtained by the spectral analysis of their corresponding temporal eigenmodes. In what follows, we examine the 3D characteristics of these turbulent coherent eigenmodes.

The typical coherent structures in turbulent flows are coherent vortices (Robinson, 2000). Here the λ_2 method (Jeong and Hussain, 1995) is adopted for identification of the coherent vortical structures. This method is based upon the notion that the cores of vortices act like an ideal rotating solid body and are characterized by local pressure minima. Jeong and Hussain (1995) showed that a local minimum of pressure exists if the second eigenvalue λ_2 of the symmetric tensor $S_{ik}S_{kj} + \Omega_{ik}\Omega_{kj}$, whose eigenvalues are ranked as $\lambda_1 \geq \lambda_2 \geq \lambda_3$, is negative. The rates of strain and rotation are defined as $S_{ij} = (\partial u_i / \partial x_j + \partial u_j / \partial x_i) / 2$ and $\Omega_{ij} = (\partial u_i / \partial x_j - \partial u_j / \partial x_i) / 2$, respectively.

The λ_2 method is first applied to the first and second spatial eigenmodes in zone 1. The isosurface of a negative λ_2 value is used to visualize the coherent vortices. Fig. 9, A and B, exhibit the side views of the vortical structures found in the respective first and second eigenmodes. The vortices extend from the laryngopharynx to the supraglottic space, and then to the glottis. The velocity vectors in the vertical planes denoted by the solid lines in Fig. 9, A and B, are displayed in Fig. 9, C and D. The front views indicate the presence of a pair of counter-rotating vortices. These vortices are not symmetric in that the first eigenmode is characterized by a clockwise-rotating vortex, whereas the second eigenmode is featured by a counter-clockwise-rotating vortex. These structures bear a resemblance to the “wake” eigenmodes or the “pulsating” Taylor-Görtler-like vortices found in an open cavity flow that are known to produce certain frequencies, sounds, and oscillations (Pastur et al., 2005; Podvin et al., 2006; Rowley and Williams, 2006). When the air flows from the laryngopharynx to the supraglottic space, the esophageal space acts as an open cavity where vortices are formed both in the cavity (approximately corresponding to the left side of the solid lines above the bifurcation in Fig. 9, A and B) and in the main-stream flow (corresponding to the right side of the lines). The frequencies of the first and second eigenmodes are 0.4167 and 1.4583 Hz, respectively (table 2). It is noted that the locations of these vortices coincide with the local TKE maximum revealed in Fig. 8, A and B.

In zone 2, the vortical structures associated with the first and second eigenmodes are exhibited in Fig. 10, A and B. The Taylor-Görtler-like vortices, which are known to appear in a curved pipe flow, are found at the concave side of the subglottic space. The contours of the corresponding v velocity and the velocity vectors in the vertical plane at $x=0$ are shown in Fig. 10, C and D, revealing the subtle difference between them. The negative v velocity (blue) of the first eigenmode is limited to above the shallow cavity. As a consequence, two positive v regions (yellow) are formed. One is located inside the cavity that forms a recirculation as indicated by the velocity vectors. The other is found near the convex side of the airway. On the other hand, the negative v velocity of the second eigenmode covers a broader region than the first eigenmode and extends into the cavity space. Both the first and second eigenmodes

have the same frequency of 10.4167 Hz (table 2). It is of note that the regions of strong fluctuations of the two eigenmodes coincide with the local maxima of the TKE contours shown in Fig. 8A.

In zone 3, the first and second eigenmodes are shown in Fig. 11. The first eigenmode appears primarily in the LMB in the form of a pair of counter-rotating vortices with one above the other as shown in Fig. 11, A and C. The second eigenmode appears in both the LMB and the RMB also in the form of a pair of counter-rotating vortices with one lateral to the other as shown in Fig. 11, B and D. It is noted that the first eigenmode in zone 3 has the same frequency as the first eigenmode in zone 1 (see table 2), but the physical correlation between them is unclear. The counter-rotating vortices in zone 3 are transient in nature with certain frequencies unlike the quasi-steady laminar flow in case 2. Consequently, these vortices do not appear clearly in the mean velocity field. This explains why the counter-rotating vortices in case 2 in the mean field (Fig. 6E) are more defined than case 1 (Fig. 6B).

4. DISCUSSION

The current study has demonstrated one of the first steps towards using patient-specific data on airway dimensions and prediction of regional airflow characteristics to phenotypically describe that subject; this approach has already been reported for vascular structures (Birchall et al., 2006). We have demonstrated the process of constructing a realistic subject-specific upper respiratory tract geometry and CFD mesh from MDCT images that includes a mouth piece, the mouth, the oropharynx, the larynx, and the intra-thoracic airways of ~6 generations. Application of the geometry to simulating airflow in the lungs and studying the effect of the laryngeal jet and turbulence concludes that the mean velocity in the trachea is not of parabolic type, but exhibits a curved sheet-like shape; the turbulence intensity is about 20% in the subglottic space and ranges from 5% to 20% in the main-stem bronchi; the RUL and LUL are less affected by the laryngeal jet; and the maximum TKE is located in the subglottic space between the vocal cords and the entrance of the trachea. In typical high-turbulence flows, the turbulence intensity ranges from 5% to 20%. Thus, the effect of turbulence on the airflow in these regions of the airways is significant. Furthermore, the presence of turbulence in the subglottic space increases the localised tracheal wall shear stress by three folds. The study also shows that neglecting the oropharynx and larynx leads to different flow structures: velocity parabola in the trachea and negligible turbulence. A POD analysis reveals that the regions of local maximum turbulence are associated with Taylor-Görtler-like coherent vortical structures in the supraglottis and the subglottis, and with counter-rotating vortices in the main-stem bronchi. These vortices possess certain spectral signatures, which can serve as a future means of model validation, and tend to be formed in localised human airway structures that bear a resemblance to the shape of an open cavity and/or a curved pipe. Thus, it is likely that human subjects who have a curved trachea may be more easily subject to shear stress related lung diseases.

The numerical results presented here have some similarities and several important differences from previous flow experiments and CFD analyses of airflow. Results for case 2 – with no laryngeal jet – are consistent with Nowak et al. (2003) who used a symmetric Weibel model to demonstrate a velocity parabola in the trachea and counter-rotating vortical structures in the LMB and RMB, consistent with experimental results (Pedley et al., 1970). A velocity parabola and counter-rotating vortices in the LMB are also present in the MDCT-based geometry for case 2 (Fig. 6E). Results for case 2 are also consistent with the anatomical model of van Ertbruggen et al. (2005), who found that using a laminar model gave no significant differences from results using a RANS turbulence model. Their model geometry initiated at the trachea, and therefore is geometrically similar to case 2. Our finding that kinetic energy is stronger in the airways of the lower lobes is consistent with experimental measurements: Cohen et al.

(1989) measured flow distribution in human and canine tracheobronchial airway casts, extending from below the larynx to airways 1 mm in diameter and showed that the inertia of airflow carries more of the flow to airways of the lower lobes.

Our prediction of a laryngeal jet biased towards the rear wall (Fig. 5, A and B, and Fig. 6A) is in contrast to Zhang and Kleinstreuer (2004), who found it biased towards the front wall of the trachea in an idealized tubular oropharynx geometry and a 4-generation symmetric Weibel model (generation 0–3). The velocity fields in the trachea and the LMB and RMB at steady inspiration also exhibit different features from their study. There are obvious differences between the two studies that will contribute to this: Zhang and Kleinstreuer used a $k-\omega$ turbulence model in an idealized cylindrical geometry, whereas the current study employs DNS in an anatomically detailed geometry.

Kamm et al. (1986) studied the effect of a turbulent jet on gas transport during oscillatory flow. An internal air jet of 0.16 cm diameter was introduced near the midpoint of a quartz tube with 2 cm diameter and 1.4 m long. They found that axial transport of mass and energy in the far field was augmented by the turbulence as well as the flow oscillations. Although their jet is different from the laryngeal jet studied here, their study suggests that airway turbulence may affect the transport of mass and energy by turbulence fluctuations in the region far from the laryngeal jet.

Grgic et al. (2004) found that aerosol depositions in the mouth and throat are affected by intra-subject differences, but even more so by inter-subject differences. For the majority of the models studied, the mouth region, viz. the location of the tongue (Heenan et al., 2004), was the largest obstacle for the aerosols. Thus, the turbulence intensity in the mouth region might depend on the location of the tongue of the subject. In the present case, Fig. 8A shows that there exists a region of high turbulence after flow passes the front of the tongue which resembles an open cavity (the space below the tongue) and a curved channel (bounded by the upper mouth geometry). However, as the air reaches the oropharynx and laryngopharynx, the turbulence intensity reduces due to expansion in volume. Thus the turbulence produced in the mouth region would have modest effect on the flow in the intra-thoracic airways.

In summary, this work demonstrates the feasibility and value of utilizing a subject-specific MDCT-based lung model together with an advanced parallel computational technique for the study of pulmonary airflow. The comparison of flow characteristics in models that include or neglect the mouth-oropharynx-larynx suggest that simple inlet boundary conditions do not adequately represent the effect of the upper airway structures, affecting the estimate of flow through several generations of airway and the tracheal wall shear stress. The methodologies and techniques presented here can be further applied to other healthy and diseased human subjects for inter-subject statistical analysis and to better understand variations in regional air flow that might contribute to understanding the evolution of many common lung diseases, and the response of the lung to inhaled medication or air pollutants.

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APPENDIX A: MODEL VALIDATION AND SGS ESTIMATION

Although DNS with a dense mesh is adopted for this study, there is a need to estimate the uncertainty of resolving all the dissipative scales. For this purpose, we repeat the lung simulation using LES with a SGS model developed by Vreman (2004), which can handle not only turbulent flow but also transitional flow. First, the in-house LES is demonstrated to accurately predict the near-wall logarithmic mean velocity profile in a turbulent channel flow (not shown). Then, both DNS and LES approaches are applied to the same lung model on a mesh of 431,476 nodes and 2,081,097 elements. Thus, the only difference between them is caused by the Vreman SGS model that represents the unresolved SGS eddies. The results show that the relative L1 norm of TKE between DNS and LES solutions is 13.6% and the relative L1 norm of the mean speed between them is 2.64%. The difference in TKE is within the typical range of a LES model, and serves as a quantitative measure of the numerical uncertainty in the current simulation.

Fig. 1.
The upper respiratory tract for a human subject: top view of the mouth (A), inside oblique view of A cutting through A along the white line (B), front view of the CT-based human airway (C), oblique view of C (D).

Fig. 2.

The entire geometry used for case 1: front view (A) and side view (B), units m. Z1, Z2, and Z3 correspond to zones 1, 2, and 3, respectively, given in table 2.

Fig. 3.
A snapshot of the surface mesh (A), and the 3D interior mesh intersecting with a horizontal plane at $y = 0$ m (B).

Fig. 4.

Time history of velocity (u, v, w) in m/s and pressure p/ρ in m^2/s^2 at the point of $(x, y, z) = (0.00, 0.040, 0.011)$ m, which is in the vicinity of the centerline of the trachea. The solid horizontal lines represent the mean values of $(\bar{u}, \bar{v}, \bar{w}, \bar{p}/\rho) = (-0.0609, -2.3983, -0.8910, -5.4359)$.

Fig. 5. Isosurface of mean speed at 2 m/s: front view of case 1 (A), side view of case 1 (B), front view of case 2 (C), side view of case 2 (D). S.1, S.2 and S.3 are the stations whose velocity vectors are displayed in Fig. 6. The arrow marks the location of flow separation and recirculation.

Fig. 6. Velocity vector field and contours of speed at station S.1 (A, D), S.2 (B, E), S.3 (C, F) for case 1 and case 2, respectively. Stations S.1, S.2 and S.3 are marked in Fig. 4A.

Fig. 7. Contours of kinetic energy of the mean velocity, MKE in m²/s² (A, D), turbulent kinetic energy, TKE in m²/s² (B, E), and the turbulence intensity (C, F) in a vertical plane at $z \approx 0$ m, cutting through trachea and major bronchial airways. The upper panel belongs to case 1, whereas the lower panel belongs to case 2.

Fig. 8. Contours of turbulent kinetic energy, TKE in m^2/s^2 (A) in a vertical plane of $x=0$ m, and in horizontal planes of $y=0.06$ m (B), 0.04 m (C), 0.02 m (D), and 0 m (E).

Fig. 9. Vortical structures in zone 1 identified by the isosurface of $\lambda_2 = -5$: side view of the first eigenmode (A), side view of the second eigenmode (B), front view of the first eigenmode (C), front view of the second eigenmode (D). The velocity vector fields in the z-plane along the solid lines in A and B are displayed in C and D.

Fig. 10.

Vortical structures in zone 2 identified by the isosurface of $\lambda_2 = -5$ and contours of v velocity fluctuation: side view of the first eigenmode (A), side view of the second eigenmode (B), v -contours of the first eigenmode (C), v -contours of the second eigenmode (D). The velocity vector fields in the plane of $x=0$ are displayed in C and D.

Fig. 11. Vortical structures in zone 3 identified by the isosurface of $\lambda_2 = -5$: side view of the first eigenmode (A), side view of the second eigenmode (B), top view of the first eigenmode (C), top view of the second eigenmode (D).

Table 1

Analysis of the airway geometry of human subject H-869

Name	avgArea	centerLineLength	avgDiameter	Generation
Trachea	160.9	267.4	14.3	0
LMB	59.7	50.6	8.7	1
TriLUL	72.8	10.0	9.6	2
LB1	10.9	16.8	3.7	5
LB2	10.9	8.0	3.7	5
LB3	20.2	6.6	5.1	4
LB4	11.8	11.6	3.9	4
LB5	9.2	20.9	3.4	4
LLB6	63.7	12.9	9.0	2
LB6	28.4	9.3	6.0	3
TriLLB	46.1	8.0	7.7	4
LB8	18.2	14.6	4.8	4
LB9	15.1	7.9	4.4	5
LB10	15.5	8.1	4.4	4
RMB	134.0	22.2	13.1	1
TriRUL	61.7	16.3	8.9	2
RB1	21.1	11.0	5.2	3
RB2	17.4	13.9	4.7	4
RB3	11.7	29.8	3.9	4
BronInt	79.8	31.8	10.1	2
RB4	19.1	7.4	4.9	4
RB5	7.5	10.7	3.1	4
RB6	24.6	10.9	5.6	4
RLL7	45.2	11.0	7.6	3
RB7	6.6	12.5	2.9	4
RB8	18.0	14.7	4.8	5
RB9	13.2	15.4	4.1	6
RB10	18.4	5.0	4.8	6

avgArea, average area in mm²; centerLineLength, the length of the 1D centerline in mm; avgDiameter, average diameter in mm; generation, the generation number of the airway branch.

Table 2

POD Analysis

Name	Region	TKE/MKE	Spatial eigenmode	Frequency (Hz)	Period (s)	TKE fraction
Zone 1	laryngopharynx, supraglottis & glottis	0.067	1 st	0.4167	2.4	0.0754
Zone 2	Subglottis & trachea	0.056	2 nd	1.4583	0.6857	0.0426
Zone 3	LMB & RMB	0.029	1 st	10.4167	0.096	0.1553
			2 nd	10.4167	0.096	0.1100
			1 st	0.4167	2.4	0.1495
			2 nd	3.3333	0.3	0.1034