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Direct numerical simulations of flow in realistic mouth-throat geometries

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ABSTRACT

The flow in a set of four realistic mouth-throat geometries at a flow rate of 30 L/min is studied in order to determine the effect of intrasubject and intersubject variations on the mean flow patterns and the turbulence fluctuations. Direct numerical simulations (DNS) are performed, which fully resolve all the scales in the flow, without requiring a turbulence model. An immersed boundary method is applied on curvilinear grids which simplifies the task of grid generation for the complex extrathoracic geometries and allows the use of a structured grid solver which increases the efficiency of the numerical scheme. Inspection of the mean, responsible for the convective transport of particles, and the fluctuating component of velocity, responsible for turbulent dispersion, allows us to explain in vitro deposition data in the literature obtained in the same mouththroat models. The results provide insight as to how geometric variation affects aerosol deposition and explain the scatter in deposition data observed in the literature. Geometric variation is shown to have a large impact on both the mean velocity profiles and the turbulence intensities. Examination of the flow fields in the various mouththroat geometries allows us to address the origin of the dependence of deposition on Reynolds number, and provide the physical significance of the empirical Reynolds number correction previously proposed in the literature.

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1. Introduction

Aerosolized delivery of drugs to the lungs has been used for decades to treat a number of respiratory diseases such as asthma, chronic obstructive pulmonary disease (COPD), cystic fibrosis and pulmonary infections. The aerosol is generally inhaled through the mouth as it is more effective than the nasal route, allowing a higher dose to penetrate through the throat and into the lungs. For effective drug delivery, the aerosol must reach the target site within the lung. Often however, significant losses are experienced in the extrathoracic airways leading to very low pulmonary deposition. Aerosol deposition is highly dependent on the flow in the extrathoracic losses and optimize pulmonary drug delivery. To this end, direct numerical simulations (DNS) have been performed in realistic mouth-throat geometries, providing an accurate representation of the turbulent flow fields. This has allowed us to examine the effect of geometric variation on the mean flow characteristics as well as the turbulence intensity, both of which affect deposition, and to relate the flow fields to *in vitro* deposition patterns in the same models, carried out by Grgic et al. (2004b).







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A number of in vivo (Chan & Lippmann, 1980; Dunbar et al., 2002; Emmett & Aitken, 1982; Foord et al., 1978; Stahlhofen et al., 1980, 1981; Svartengren et al., 1994; Walsh et al., 1977) and in vitro studies (Cheng et al., 1999, 2001; DeHaan & Finlay, 2004; Grgic et al., 2004a, 2004b; Heenan et al., 2004; Lin et al., 2001; Shinneeb & Pollard, 2012; Zhang et al., 2007; Zhou et al., 2011) have been conducted in order to develop an understanding of the flow and particle dynamics in the extrathoracic airways. In vivo experiments are costly and complex to perform, and accurate results are difficult to obtain due to spatial resolution and tissue attenuation limit (Grgic et al., 2004b). In addition, flow visualization cannot be performed. In vitro measurements are relatively easier. However, most of these studies have focused solely on deposition. Grgic et al. (2004a) and Heenan et al. (2003, 2004) conducted particle image velocimetry (PIV) measurements in order to visualize the flow. This allowed comparison of the deposition patterns with the flow field, showing a strong correlation between deposition levels and local velocity magnitude and flow curvature. However, obtaining PIV measurements in small, closed, complex geometries presents many difficulties. In addition, PIV is inherently noisy and suffers from limited resolution, so it can only capture the larger scale turbulent fluctuations. The measurements performed were also limited to the central sagittal plane due to contamination from the out-of-plane velocity component. More recently Shinneeb & Pollard (2012) carried out PIV measurements in coronal planes across the pharynx and larynx as well, in order to gain an understanding on the characteristics of the turbulent flow. Their results showed that the flow is strongly threedimensional, and that a large number of vortical structures occur in the pharynx/larynx region, which are deformed and torn apart by bursting events. However, stereo PIV commonly used in the literature can only provide 2D data. The recently developed tomographic PIV technique can obtain 3D measurements but has not to date been applied to studies of the flow in the extrathoracic airways. Numerical simulations provide an alternative to PIV and can yield a more accurate and a more detailed representation of the flow.

In the last decade, computational fluid dynamics (CFD) of the flow and the particle trajectories in the extrathoracic airways has become possible, and offers a non-invasive and cost-effective alternative to *in vivo* and *in vitro* testing. A number of Reynolds-averaged Navier–Stokes (RANS) (Heenan et al., 2003; Jayaraju et al., 2007; Kleinstreuer & Zhang, 2003; Matida et al., 2004; Sandeau et al., 2010; Zhang et al., 2002) and large eddy simulation (LES) studies (Cui & Gutheil, 2011; Debhi, 2011; Jayaraju et al., 2008; Matida et al., 2006;) have been reported in the literature. However, accurate prediction of the flow field remains a challenge due to the complexity of the flow in the extrathoracic airways and the limitations of RANS and LES turbulence models. More recently, the first direct numerical simulations in an idealized mouth–throat geometry were reported by Ball et al. (2008). The authors used a lattice Boltzmann method and demonstrated closer agreement with experimental results than RANS models.

Studies which have focused on accurately modelling the geometry have employed RANS turbulence models (Jayaraju et al., 2007; Sandeau et al., 2010) which do not resolve any of the scales in the flow, but rather model the fluctuations, usually based on empirical data obtained from canonical and often equilibrium flows. The flow in the complex extrathoracic airways differs significantly from a canonical duct flow however, and the inaccurate modelling of the fluctuations, which cause dispersion, affects the prediction of deposition. The effect is more significant for the smaller particles whose trajectories are considerably influenced by the fluctuations in the flow. On the other hand, LES which resolves the large scales in the flow and can therefore better predict turbulent dispersion, has been performed on simplified representations of the models (Cui & Gutheil, 2011; Debhi, 2011; Jayaraju et al., 2008; Matida et al., 2006). Whereas Jayaraju et al. (2008) found considerable improvement in predicting deposition for smaller particles and Cui & Gutheil (2011) showed better predictions particularly in the transitional regime using LES over RANS, Debhi (2011) obtained comparable accuracy between RANS and LES models. In addition, experiments have demonstrated the large effect that geometric complexity has on the flow, and hence deposition (Grgic et al., 2004b; Heenan et al., 2004). Therefore the simplified geometries adopted in earlier work is not sufficient. To date, there has not been a complete study including both a realistic geometry and a realistic representation of the turbulent field.

The importance of understanding and accurately capturing the flow dynamics in the extrathoracic airways is further supported by the dependence of deposition on Reynolds number, *Re*. This dependence was first observed by Grgic et al. (2004a) in *in vitro* experiments in an idealized geometry. Previously, deposition had been reported in terms of its dependence on Stokes number, *Stk*, alone. However, keeping the Stokes number constant and varying the Reynolds number, *Re*, Grgic et al. (2004a) observed an increase in deposition with *Re*. Based on PIV measurements, they were able to gain insight into this dependence and attributed it to the difference in velocity profile at different flow rates. Deposition efficiency was shown to depend on *Stk Reⁿ*. This scaling leads to better collapse of extrathoracic deposition onto a single curve, as opposed to the Stokes number alone. However, the physical significance of this Reynolds number correction was not explained. Examination of the flow fields in a number of realistic mouth–throat geometries allows us to address the origin of this Reynolds number dependence.

The present work is the first set of direct numerical simulations of the flow in realistic extrathoracic airways. Through realistic inflow conditions, geometric representation of the airways, and accurate solution of the flow field which is fully resolved, this study allows us to evaluate the effect of geometric variation on the mean flow as well as the turbulent fluctuations. Relating the flow fields to *in vitro* deposition data from the literature provides insight as to how geometric variation affects aerosol deposition, and helps to explain the scatter in deposition data reported in the literature. Finally, we explain the physical significance of the Reynolds number effect on deposition.

The paper is organized as follows: The geometries and the flow parameters used in this study are presented in Section 2. In Section 3, the numerical method is described in detail. In Section 4, the flow fields in the various mouth-throat

geometries are presented and the effect of intrasubject and intersubject variations on the mean flow and the turbulence intensity is examined. The flow fields are used to explain the *in vitro* deposition data of Grgic et al. (2004b), obtained in the same geometries. The derivation of the Reynolds number dependence of deposition is given next. Finally, Section 5 is a summary of the work.

2. Mouth-throat geometries and flow parameters

A set of four physiologically realistic mouth and throat geometries were used in this study. It is a subset of the geometries used by Grgic et al. (2004b) for their *in vitro* measurements. The anatomically accurate models were obtained using magnetic resonance imaging (MRI). The methodology is explained in detail by McRobbie et al. (2003). The MRI scans were converted to 3D volume files from which STL models were generated. The geometries can be divided into four sub-regions (see Fig. 1):

- (1) the mouth region from the back of the teeth to the soft palate;
- (2) the nasopharynx region incorporating the nasal airways to the tip of the epiglottis;
- (3) the larynx, from the tip of the epiglottis to just below the vocal cords;
- (4) the trachea to a point two vertebrae below the vocal cords.

The geometries studied here are denoted S1b, S1a, S2 and S4, in keeping with the labels used by Grgic et al. (2004b). They are shown in Fig. 2. Cases S1b and S1a represent the same subject and correspond to different configurations: In S1b, the tongue is in the forward position touching the back of the teeth, whereas in S1a, the tongue is pulled back creating a large mouth opening and reducing the size of the nasopharynx. Models S2 and S4 belong to different individuals, both with large oral cavities. In S2, the mouth narrows at the back and the pharynx is wider. Subject S4 has a wider mouth and a narrow pharynx with a bending angle close to 90°. The choice of geometries allows us to investigate the effect of both intrasubject and intersubject variations on the flow, and to explain the dependence of particle deposition on Reynolds number, as reported in the literature.

The main dimensions of the models are listed in Table 1. In order to calculate the sagittal length, *L*, the geometries were split along the central sagittal plane. Because the geometries are not symmetrical, the mid-plane was chosen such that each of the two halves of the geometry contained approximately half the volume of the model. Once cut, the path line along the centre of the geometry was measured on that plane in order to determine the length. Assuming a circular mean



Fig. 1. Sub-regions of the mouth-throat shown on the central sagittal plane.



Fig. 2. Geometries used in the DNS: (a) S1b, (b) S1a, (c) S2, and (d) S4.

Table	1
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Dimensions of the mouth and throat geometries.

Model	S1b	S1a	S2	S4
D _{inlet} (cm)	0.83	1.30	2.30	2.30
Volume (cm ³)	38.63	51.56	81.73	84.20
Length (cm)	18.90	19.10	18.60	19.10
D _{mean} (cm)	1.61	1.85	2.37	2.37

Table 2

Flow parameters in the mouth and throat geometries.

Model	S1b	S1a	S2	S4
U _{inlet} (m/s)	3.92	3.77	1.20	1.20
U _{mean} (m/s)	2.74	1.88	1.13	1.13
Re _{inlet}	3292	3222	1815	1815
Re _{mean}	2744	2262	1761	1761

cross-sectional area, an equivalent mean diameter was computed for each model according to

$$D_{\rm mean} = 2\sqrt{\frac{V}{\pi L}},$$

where *V* is the volume of the geometry.

Direct numerical simulations in the four geometries were carried out at a flow rate Q = 30 L/min. The main flow parameters in the different models are summarized in Table 2. The mean velocity is determined from the volume flow rate and the mean cross-sectional area according to

$$U_{\rm mean} = \frac{QL}{V} \tag{2}$$

and the Reynolds number based on the mean diameter and the mean velocity in the mouth-throat geometry is given by

$$Re_{\rm mean} = \frac{D_{\rm mean}U_{\rm mean}}{v},\tag{3}$$

where v is the kinematic viscosity of the fluid.

3. Numerical method

Due to the complexity of the mouth-throat geometries, an immersed boundary (IB) method is employed. IB methods employ structured, non-conforming grids and incorporate the boundary conditions by modifying the Navier–Stokes equations near the wall of the geometry. This approach greatly simplifies the task of grid generation and discretization of the governing equations, and eliminates the problems associated with grid quality that exist with boundary-fitted grid techniques. The IB approach also allows the use of a structured grid solver, which is advantageous from the point of view of computational efficiency and scalability on high performance computing facilities, in comparison to unstructured grid methods.

(1)



Fig. 3. Grids for model S1a. (a) Cartesian grid. Every eighth grid line in x and y has been plotted. (b) Curvilinear grid. Every fourth grid line in ξ and eighth grid line in η .

In order to accurately resolve the flow, a high grid resolution is required inside the geometries. Due to the shape of the extrathoracic airways, the use of Cartesian grids which are commonly adopted in IB methods leads to many unused grid points outside the flow domain (see Fig. 3a). Even when grid stretching is applied, it is difficult to cluster the points efficiently inside the geometry. For turbulent flow, which is the case at the flow rate considered herein, the resolution requirements become prohibitively expensive. A more efficient alternative is therefore to adopt a curvilinear grid that roughly follows the shape of the geometry. This greatly reduces the number of points outside the geometry, thus allowing for much higher resolution within the geometries than the Cartesian grid case (see Fig. 3b). An added advantage of the curvilinear mesh is that the grid lines are approximately aligned with streamlines, which is favourable from a numerical accuracy point of view as this tends to reduce numerical diffusive errors.

Initial computations were performed on a grid with 14×10^6 cells $(385 \times 193 \times 193$ grid points). Based on the results from the coarse mesh computations, the grid was refined in the streamwise ξ , cross-stream η and spanwise z directions. The final, fine mesh computation included 42×10^6 cells $(513 \times 321 \times 257 \text{ grid points})$, with uniform grid spacing in the spanwise direction, $\Delta z = 0.0094$, and hyperbolic tangent stretching in the streamwise and wall-normal directions in order to minimize the number of points outside the geometry and provide adequate resolution near the walls, $0.01 < \Delta \xi < 0.06$ (near the outflow) and $0.02 < \Delta \eta < 0.008$. Using the friction velocity at the inlet pipe, this corresponds to $\Delta z^+ = 3.12$, $3.32 < \Delta \xi^+ < 19.9$ (near the outflow) and $0.66 < \Delta \eta^+ < 2.65$ in wall units, which falls in the range typically used in the literature for turbulent internal flows. The time step is $\Delta t^+ = 0.024$, which is significantly smaller than the Kolmogorov time scale and hence adequate for time-resolved computations. Choi & Moin (1994) demonstrated accurate prediction of turbulence statistics for $\Delta t^+ < 0.4$. The overall run-time for a simulation on 128 processors was approximately 300 h, including the initial time to remove the transient and the time to compute statistics.

The no-slip condition at the immersed boundary is applied via a direct forcing approach similar to that by Kim et al. (2001), which consists in adding a momentum forcing term, f, on the boundary and inside the solid domain. The forcing ensures that the velocity at the surface of the immersed body satisfies the boundary conditions. A mass source/sink, q, is applied to cells containing the immersed boundary in order to ensure mass conservation. The governing equations in non-dimensional form are therefore given by

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\nabla p + \frac{1}{Re_{\text{mean}}} \nabla^2 \boldsymbol{u} + \boldsymbol{f}, \tag{4}$$

$$\nabla \cdot \boldsymbol{u} - \boldsymbol{q} = \boldsymbol{0},\tag{5}$$

where $\mathbf{u} = (u, v, w)$ is the velocity vector, p is the pressure, \mathbf{f} is the momentum forcing vector and q is the mass source/sink. The equations are solved on a staggered curvilinear grid using a finite volume scheme, following the method described in Rosenfeld et al. (1991). Time integration is performed with a second-order fractional step method: First, a provisional velocity $\hat{\mathbf{u}}$ is computed and then a pseudo-pressure, ϕ , is used to correct the provisional velocity field so that the continuity equation is satisfied at each computational time step (Kim & Moin, 1985).

The diffusive terms are treated implicitly using the Crank–Nicholson scheme, in order to avoid the restrictive viscous stability condition, $\Delta t \leq \Delta x^2/\nu$. The non-linear convective terms are treated explicitly using an Adams–Bashforth scheme. The discretized equations are given by

$$\frac{\hat{\boldsymbol{u}} - \boldsymbol{u}^{n-1}}{\Delta t} = -(\gamma N(\boldsymbol{u}^{n-1}) + \delta N(\boldsymbol{u}^{n-2})) - \nabla p^{n-1} + \frac{1}{Re_{\text{mean}}} (\alpha L(\hat{\boldsymbol{u}}) + \beta L(\boldsymbol{u}^{n-1})) + \boldsymbol{f}^n,$$
(6)

$$\nabla^2 \phi^n = \frac{1}{\Delta t} (\nabla \cdot \hat{\boldsymbol{u}} - q^n), \tag{7}$$

$$\boldsymbol{u}^n = \hat{\boldsymbol{u}} - \Delta t \nabla \phi^n, \tag{8}$$

$$p^n = p^{n-1} + \phi^n,\tag{9}$$

where $N(\mathbf{u})$ are the convective terms, $L(\mathbf{u})$ are the implicit diffusive terms and $(\alpha, \beta, \gamma, \delta)$ are weighting coefficients which depend on the numerical scheme adopted. In our case, $\alpha = 3/2$, $\beta = -1/2$ for the Adams–Bashforth scheme and $\gamma = \delta = 1/2$ for the Crank–Nicholson scheme.

The inflow condition: The flow at the inlet to the computational domain was designed based on the Reynolds number, in order to match the experimental flow setup. For geometries S2 and S4, since the Reynolds number is in the laminar regime, a parabolic velocity profile is prescribed at the inlet. For S1a and S1b, where the flow in the inlet tube is turbulent, accurate turbulent inflow conditions are required. These were obtained from a separate direct numerical simulation of pipe flow at the Reynolds number reported in the experiments.

The length of the pipe is $L_x = 5D_{inlet}$, which is sufficiently long to include the largest structures in the flow (Eggels et al., 1994). A 256 × 128 × 64 grid is employed, with uniform spacing in the streamwise and circumferential directions, $r\Delta x^+ = 4.55$, $(\Delta\theta)^+ = 5.72$, and stretching in the radial direction in order to provide adequate resolution near the walls, $0.09 \le \Delta r^+ \le 4.96$. Similar grid resolutions have previously been adopted in the literature (Eggels et al., 1994; Kim et al., 1987). Starting from a laminar flow field with superimposed initial fluctuations, fully developed turbulence is obtained after ten flow-through times.

By invoking Taylor's et al. (1938) hypothesis, convective spatial fluctuations can be interpreted as temporal fluctuations. In this manner, the axial pipe coordinate can be transformed into a time coordinate. The first cross-sectional plane from the turbulent pipe flow is applied as an inflow condition to the mouth at the initial time, and the time-dependence of the inflow is emulated by sweeping through planes along the pipe axis. The mean velocity profile and the mean turbulence intensities at the inlet are shown in Fig. 4.

The outflow condition: At the outflow boundary, a convective condition is applied. This is given by

$$\frac{\partial \boldsymbol{u}}{\partial t} = -c \frac{\partial \boldsymbol{u}}{\partial n}, \quad c < 0, \tag{10}$$

where c is the convective velocity, chosen to be the bulk velocity at the outlet, and n is the direction normal to the exit plane. An extension approximately two mean diameters long was added to the outlet of the mouth-throat geometries for two reasons: Firstly, the extended domain ensures that any inaccuracies in estimating the outflow conditions are not propagated upstream into the region of interest. Secondly, the extension ensures that the outflow plane is downstream of any separation zone.



Fig. 4. (a) Mean streamwise velocity \overline{u} normalized by the inlet bulk velocity U_{inlet} . (b) Turbulence intensities normalized by the inlet bulk velocity: —, u_{rms} ; – - -, v_{rms} ; – - -, w_{rms} .



Fig. 5. Contours of (a) instantaneous velocity magnitude and (b) fluctuation magnitude in geometry S1a.

The instantaneous velocity field u comprises a mean component \overline{u} and a fluctuating component u':

$$u = \overline{u} + u'$$
.

Snapshots of the instantaneous velocity magnitude and the magnitude of fluctuations in one of the geometries are shown in Fig. 5. It illustrates the turbulent nature of the flow. The mean velocity is responsible for the convective transport of aerosol particles, whereas the fluctuations are responsible for turbulent dispersion. Understanding the deposition of particles in the extrathoracic airways therefore requires inspection of both the mean and the fluctuating components of the velocity.

The mean velocities and root-mean-square of the fluctuating components are computed with a running average in time:

$$\overline{\boldsymbol{u}} = \frac{1}{T} \int_0^T \boldsymbol{u} \, dt,\tag{12}$$

$$\boldsymbol{u}_{\rm rms} = (\overline{\boldsymbol{u}^{\prime 2}})^{1/2} = \left(\frac{1}{T} \int_0^T \boldsymbol{u}^2 \, dt - \overline{\boldsymbol{u}}^2\right)^{1/2},\tag{13}$$

where *T* is the time period for statistical convergence. We study the effects of intrasubject and intersubject variations on the flow field by comparison of the mean flow patterns and the mean turbulent kinetic energy per unit mass

$$k = \frac{1}{2}(\overline{u^{\prime 2}} + \overline{v^{\prime 2}} + \overline{w^{\prime 2}})$$

across geometries.

4. Results and discussion

4.1. Intrasubject variation

Comparison between geometries S1b and S1a shows how intrasubject variation can account for significant differences in the flow field. Figs. 6a and 7a show contours of the mean velocity magnitude in the central sagittal plane and at various cross-sections in models S1a and S1b respectively. Two-dimensional streamlines in the corresponding planes are plotted in Figs. 6b and 7b respectively.

In S1b, the velocity profiles in the mouth are highly skewed towards the inner wall due to the airway curvature (A1–A2). The flow accelerates at the back of the mouth due to the restriction in cross-sectional area, developing a pharyngeal jet which impinges onto the posterior wall (B1–B2). Due to the bend in the airway, the flow shifts towards the outer wall, separating from the inner wall and leading to a recirculation region. The maximum velocity then decreases as the larynx expands in the spanwise direction, and flow moves into the lateral expansions (C1–C2). A small recirculation region at the posterior side of the exit to the trachea can be observed under the 'sharp step' in the larynx (upstream of E1–E2).

Due to the wider oral cavity in model S1a, there is no pharyngeal jet (B1–B2). As a result, the velocity in the pharynx is lower and the flow does not separate from the inner wall. Instead, the flow accelerates further downstream resulting in higher velocities in the larynx (D1–D2), due to the narrower nasopharynx than in S1b. This in turn leads to a larger separation region near the outer wall of the trachea (E1–E2).

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Fig. 6. (a) Contours of mean velocity magnitude and (b) 2D streamlines in the central sagittal plane and at various cross-sections of geometry S1b.

Heenan et al. (2004) conducted PIV measurements of the flow in the same geometries at both Q=30 and 90 L/min. They asserted that the flow was qualitatively similar for the two flow rates, and discussed the case with Q=90 L/min in detail. Therefore, their results can be used for qualitative comparison of the main flow features. The PIV measurements in both geometries display the same mean flow characteristics as the flow fields presented herein. In S1b, both DNS and PIV results show the existence of a pharyngeal jet impinging on the posterior wall in the upper pharynx (Fig. 6 herein and Fig. 4 by Heenan et al., 2004). In S1a, we note the absence of a jet in both experimental and numerical results, and an increase in the velocity further downstream in the larynx (Fig. 7 herein and Fig. 6 by Heenan et al., 2004). The only discrepancy between the two sets of results is in the oral cavity in S1a, where the impingement of the inlet flow on the front of the tongue is inappreciable in the PIV measurements due to the wider inlet pipe used in the experiments. However, as can be seen from the results and has also previously been reported in the literature, the inflow shows no appreciable effect on the flow downstream (Ball et al., 2008). Finally, the separated shear layer in the trachea of S1a was not reported by Heenan et al. (2004) as their PIV measurements focused on the upstream region of the flow.

In addition to the agreement with the PIV data in the central sagittal plane, the current computations have provided a high-resolution representation of the flow field throughout the extrathoracic airways, for example in the coronal crosssections discussed above. The direct numerical simulations also provide accurate characterization of the turbulence. Contours of the turbulent kinetic energy per unit mass in S1b and S1a are shown in Fig. 8a and b respectively. The plots show that the turbulence intensity is higher in model S1a, even though the Reynolds number is lower. This is due to the inflow condition and the geometry of the airways. The flow in the mouth in S1b is similar to pipe flow, whereas in S1a a jet from the inlet pipe impinges against the tongue. Separation occurs at the upper wall due to the wide oral cavity, and under the jet where the flow resembles that over a backward-facing step. Higher levels of turbulent kinetic energy can be observed near the regions of separation. The maximum kinetic energy in S1b occurs in the upper pharynx near the jet, and



Fig. 7. (a) Contours of mean velocity magnitude and (b) 2D streamlines in the central sagittal plane and at various cross-sections of geometry S1a.

in S1a, in the larynx. High values of *k* can also be observed downstream of the vocal cords (see the sagittal plane in Fig. 8a). These are locations where separated shear layers exist. Generally, turbulence is strongest where mean shear is largest.

The flow fields can be used to explain the *in vitro* deposition results of Grgic et al. (2004a). The deposition fractions in the different regions of geometries S1a and S1b are given in Table 3. For all three particle sizes the main difference between the two geometries is the increased pharyngeal deposition in S1b. This is due to the pharyngeal jet, which causes particles to deposit on the posterior wall of the upper pharynx via impaction.

Deposition levels for the smallest $3 \mu m$) and the largest (6.5 μm) particles are very similar in both geometries. For the smallest particles, slightly higher deposition in the mouth and pharynx is observed in S1b. Not only do particles deposit via impaction at the back of the mouth and the upper pharynx, but in addition, the high levels of turbulence intensity on either side of the jet (see Fig. 8b) cause particle dispersion, causing small particles travelling near the wall in the upper pharynx to deposit. In S1a, high turbulent kinetic energy can be observed in the larynx, which explains the slightly higher deposition (via dispersion) in this region, compared to S1b. It is clear that both the mean flow characteristics and the velocity fluctuations play a role in the deposition of the small particles.

Large particles are less influenced by the velocity fluctuations and therefore the main deposition mechanism is impaction. Oral deposition in S1a occurs at the front of the tongue where the incoming flow from the inlet pipe impinges, whereas in S1b it occurs mainly at the back of the mouth due to the high velocities and the airway curvature. For the medium-sized particles, deposition in the mouth, pharynx and larynx is significantly higher in S1b, via impaction due to the pharyngeal jet. The fact that this significant difference in deposition between S1a and S1b is not also observed for the largest-sized particles is somewhat anomalous, as mentioned by Grgic et al. (2004a), who cited the large variation in regional deposition and flow field measurements reported by Heenan et al. (2004). Deposition in the trachea is higher in S1a due to the high-velocity separated shear layer that forms at the sharp step in the larynx (see location D1–D2 in Fig. 6).

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Fig. 8. Contours of mean turbulent kinetic energy in the central sagittal plane and at various cross-sections of (a) geometry S1b and (b) geometry S1a.

Table 3Deposition in the different regions of the S1a and S1b geometries, given as a percentage of aerosol entering the mouth (Grgic et al., 2004a).

Particle size (µm)	Geometry	Regions	Regions			
		Mouth (%)	Pharynx (%)	Larynx (%)	Trachea (%)	Total (%)
3.0	S1b S1a	$\begin{array}{c} 0.56 \pm 0.12 \\ 0.39 \pm 0.04 \end{array}$	$\begin{array}{c} 0.62 \pm 0.07 \\ 0.22 \pm 0.01 \end{array}$	$\begin{array}{c} 0.38 \pm 0.07 \\ 0.47 \pm 0.06 \end{array}$	$\begin{array}{c} 0.17 \pm 0.06 \\ 0.15 \pm 0.01 \end{array}$	$\begin{array}{c} 1.73 \pm 0.36 \\ 1.23 \pm 0.12 \end{array}$
5.0	S1b S1a	$\begin{array}{c} 11.58 \pm 2.31 \\ 2.86 \pm 0.50 \end{array}$	$\begin{array}{c} 11.68 \pm 1.39 \\ 2.14 \pm 0.66 \end{array}$	$\begin{array}{c} 10.06 \pm 2.47 \\ 5.71 \pm 1.47 \end{array}$	$\begin{array}{c} 1.33 \pm 0.32 \\ 1.10 \pm 0.34 \end{array}$	$\begin{array}{c} 34.63 \pm 2.29 \\ 11.81 \pm 2.56 \end{array}$
6.5	S1b S1a	$\begin{array}{c} 25.64 \pm 6.66 \\ 24.32 \pm 0.31 \end{array}$	$\begin{array}{c} 15.49 \pm 1.77 \\ 10.68 \pm 2.68 \end{array}$	$\begin{array}{c} 18.02 \pm 7.59 \\ 20.96 \pm 0.82 \end{array}$	$\begin{array}{c} 2.90 \pm 2.25 \\ 6.23 \pm 0.74 \end{array}$	$\begin{array}{c} 62.05 \pm 2.63 \\ 62.19 \pm 3.50 \end{array}$

4.2. Intersubject variation

Geometries S2 and S4 have the same inlet diameter and the same mean Reynolds number, making the comparison between the two geometries a good test of the effect of geometric variation on the flow field. Both geometries are considerably different to S1a and S1b. This results in significant differences in the flow fields, which can be observed in the velocity contours shown in Figs. 9a and 10a, and in the streamlines plotted in Figs. 9b and 10b. The velocities reach much higher levels when normalized by the reference speed, as the variation in the cross-sectional area is much larger. However, absolute values of velocity are lower as the geometries on average are wider (see Table 1).



Fig. 9. (a) Contours of mean velocity magnitude and (b) 2D streamlines in the central sagittal plane and at various cross-sections of geometry S2.

In S2, the velocities in the mouth are low due to the wide oral cavity, with recirculation at the top and bottom walls near the inlet. Strong secondary flow exists, as the fluid coming in from the pipe moves radially outwards to fill the wide area (A1–A2). The fluid then accelerates at the back of the mouth and upper pharynx due to the large reduction in cross-sectional area (B1–B2). An obstruction in the centre of the airway causes the flow to split into two diverging jets (C1–C2), shifting the flow towards the side walls (D1–D2). Four distinct counter-rotating vortices can be observed at this location: two main cells at the centre, and two smaller cells near the side walls. The main cells resemble Dean vortices known to appear in curved ducts as a result of centrifugal instability. Smaller secondary flow weakens and the velocity drops due to an increase in cross-sectional area (E1–E2). A small recirculation region develops near the anterior wall due to the sharp expansion. The flow in the trachea is similar to S1a, with the fluid accelerating again as it passes the sharp bend (F1–F2) and a small separation region developing near the posterior wall (G1–G2).

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Fig. 10. (a) Contours of mean velocity magnitude and (b) 2D streamlines in the central sagittal plane and at various cross-sections of geometry S4.

Similar to model S2, the velocity in the mouth of geometry S4 is low and strong secondary flow exists, due to the large oral cavity (A1–A2). The back of the mouth is wider than in S2, so velocities there are lower (B1–B2). Instead, the flow accelerates further downstream, after the sharp 90° bend into the pharynx (C1–C2). The velocity remains roughly constant throughout the pharynx as the cross-sectional area does not change appreciably. The small expansion near the anterior wall is sudden so the flow remains unaffected and attached to the posterior wall (D1–D2). A slight drop in the velocities is observed in the larynx, where the cross-sectional area is larger (E1–E2), before an increase in the trachea as the airway narrows and bends (F1–F2). The trachea is shorter and narrower than in the other geometries, therefore velocities are still high at the exit (G1–G2).

Although the inflow is laminar based on the inlet Reynolds number, the flow in both geometries transitions to turbulence at the back of the mouth, as can be seen in Fig. 11a and b. The contours of turbulent kinetic energy in S2 show much higher levels of turbulence intensity compared to all other geometries, even though the Reynolds numbers in S1a and S1b are higher. The location of maximum *k* occurs close to the core of one of the main vortices, in the upper pharynx. This is due to the strong gradients in tangential velocity inside the vortex. In S4, most of the turbulent kinetic energy is



Fig. 11. Contours of mean turbulent kinetic energy in the central sagittal plane and at various cross-sections of (a) geometry S2 and (b) geometry S4.

Table	4
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Deposition in the different regions of the S2 and S4 geometries, given as a percentage of aerosol entering the mouth (Grgic et al., 2004a).

Particle size (µm)	Geometry	Regions				
		Mouth (%)	Pharynx (%)	Larynx (%)	Trachea (%)	Total (%)
3.0	S2 S4	0.49	0.67	0.33	0.13	0 1.62
5.0	S2 S4	$\begin{array}{c} 0.93 \pm 0.31 \\ 1.31 \end{array}$	$\begin{array}{c} 0.30\pm0.08\\ 1.85\end{array}$	$\begin{array}{c} 0.33 \pm 0.02 \\ 1.49 \end{array}$	$\begin{array}{c} 0.33 \pm 0.10 \\ 0.63 \end{array}$	$\begin{array}{c} 1.89 \pm 0.39 \\ 5.28 \end{array}$
6.5	S2 S4	$\begin{array}{c} 0.66 \pm 0.72 \\ 2.46 \end{array}$	$\begin{array}{c} 0.87 \pm 0.65 \\ 6.09 \end{array}$	$\begin{array}{c} 1.73 \pm 0.15 \\ 3.99 \end{array}$	$\begin{array}{c} 2.98 \pm 0.18 \\ 1.44 \end{array}$	$\begin{array}{c} 6.24 \pm 1.68 \\ 13.98 \end{array}$

produced in the pharynx and larynx due to the separated shear layers. The maximum value of *k* occurs in the upper pharynx, between the separation region and the pharyngeal jet, where shear is highest.

The flow fields can be used to explain the *in vitro* deposition results of Grgic et al. (2004a). The *in vitro* deposition fractions in the different regions of geometries S2 and S4 are given in Table 4. Deposition is low in comparison with S1a and S1b, due to the lower flow inertia. We can see that the regional and total depositions differ between S2 and S4, despite the same Reynolds number in both geometries. For all three particle sizes, slightly higher total deposition is observed in S4. This is mainly due to the higher deposition in the pharynx and larynx, as the higher velocities and the bigger radius of curvature cause the particles to deposit via impaction. The difference is most significant for the largest particles, as they have more inertia, which causes more appreciable deviation from the streamlines. Although strong secondary flow exists in the mouth as the air coming in from the inlet pipe moves radially outwards, oral deposition in both geometries is low due to the low inflow velocity and the wide oral cavity. No deposition is observed for the smallest particles in geometry S2, despite the high levels of turbulent kinetic energy, which suggests that impaction is the main deposition mechanism for the range of particle sizes considered.

The flow results presented herein and the above discussion demonstrate the following:

- (i) The flow in the extrathoracic airways is complex. Highly asymmetric velocity profiles, complex secondary flow and regions of separation are observed in all geometries.
- (ii) Transition to turbulence occurs even if the inflow is laminar, due to the complex geometry of the airways. This transition occurs rapidly, with the flow becoming turbulent around the back of the mouth. Therefore, the effect of the inflow on the flow and the deposition in the airways is mainly confined to the oral cavity. Conventional RANS approaches are known to perform poorly in transitional flows (Stapleton et al., 2000), and careful selection of a turbulence model is required for accurate prediction of flow in the airways (Longest & Vinchurkar, 2007). DNS naturally captures transition, circumventing the need to select a particular turbulence model.
- (iii) Geometric variation has a large effect on the flow field. This variation affects the flow, and in turn the particle deposition, in two ways:
 - (a) The different shape of the airways leads to different flow patterns and hence different "hot-spots" for particle deposition. For example, even in the case of geometries S2 and S4 in which the Reynolds numbers are the same, the mean flow patterns and the levels of turbulence intensity differ. This is because the Reynolds number is based on the mean characteristic length of the geometries, but the diameters of the geometries deviate considerably from the mean in many sections of the airways.
 - (b) For a given volume flow rate, the Reynolds number is different in various geometries. This changes the mean velocity profiles and the turbulence intensities which in turn affect particle trajectories and their deposition. This Reynolds number effect is the focus of the next subsection.

4.3. Reynolds number effect

Deposition efficiency in the extrathoracic airways is commonly examined in terms of its dependence on the Stokes number, given by

$$Stk = \frac{\rho_p d_p^2 U_{\text{mean}}}{18\mu D_{\text{mean}}},\tag{14}$$

where ρ_p is the particle density, d_p is the particle diameter and μ is the dynamic viscosity of the fluid. However, experiments carried out by Grgic et al. (2004a) in an idealized geometry demonstrated that there is also a dependence of deposition on the Reynolds number. They observed that the deposition efficiency at two different flow rates lay on different curves when plotted against Stokes number, indicating a possible Reynolds number effect on deposition. For this reason, another set of experiments was carried out where Stokes number. An empirical Reynolds number correction $Re^{0.37}$ that collapsed deposition data more closely onto a single curve was proposed. Using this correlation, a number of *in vitro* experiments have been plotted against $Stk Re^{0.37}$ in the literature (see Fig. 11 in Grgic et al., 2004a), and showed good collapse. The Reynolds number dependence in the work of Grgic et al. (2004a) was motivated by empirical observations and data-fitting, but its physical significance was not explained. A theoretical, or fluid-dynamical, explanation is presented herein.

As mentioned in the previous subsection, the Reynolds number dependence is due to at least two contributing factors: (1) the difference in the mean flow characteristics and (2) the difference in turbulence intensity. This was observed in the difference in mean flow features and turbulent kinetic energy among the different geometries. Whereas the effect of the mean flow field is already taken into account in the Stokes number, the level of turbulence intensities is not. Therefore, the Stokes number only accounts for impaction as a deposition mechanism, and does not include the dispersion experienced by the particles due to turbulence fluctuations. Deposition should be plotted against a parameter that takes both

deposition mechanisms into account. Plotting against the Stokes number, which only account for impaction, contributes a reason for the scatter in deposition data which has been observed in the literature.

For canonical turbulent flows, such as channel and pipe flow, particle deposition is well documented in the literature (Kallio & Reeks, 1989; Liu & Agarwal, 1974; McLaughlin, 1989; Wang & Squires, 1996; Young & Leeming, 1997) and is generally plotted against the dimensionless particle relaxation time, τ_n^+ , given by

$$\tau_p^+ = \frac{\tau_p u_\tau^2}{v}.\tag{15}$$

Here,

$$\tau_p = \frac{\rho_p d_p^2}{18\mu}$$

is the particle relaxation time and

$$u_{\tau} = \left(\frac{\tau_{w}}{\rho}\right)^{1/2}$$

is the friction velocity, where τ_w is the wall shear stress and ρ is the fluid density.

The dimensionless particle relaxation time takes into account both impaction and turbulent diffusion, and is herein used to prove the dependence of deposition on Reynolds number. Eq. (15) can be rewritten as

$$\tau_p^+ = Stk \frac{D_{\text{mean}}}{U_{\text{mean}}} \frac{u_\tau^2}{v},\tag{16}$$

where $D_{\text{mean}}/U_{\text{mean}}$ is the mean flow time scale and v/u_{τ}^2 is the viscous time scale. Since fluctuations scale roughly with the friction velocity u_{τ} , the viscous time scale can be seen as representing the fluctuation time scale. Next, an expression for the friction velocity u_{τ} is sought in terms of *Re*.

For fully developed turbulent pipe flow, a relation between the friction velocity and the mean velocity can be obtained through the expression for the friction factor

$$f = \frac{4\tau_w}{\frac{1}{2}\rho U_{\text{mean}}^2} = 8\left(\frac{u_\tau}{U_{\text{mean}}}\right)^2.$$
(17)

Blasius (1913) derived a fit for the experimental data, given by

$$f = \frac{0.3164}{Re^n},$$
 (18)

where n=0.25, from which an expression for the friction velocity can be obtained

$$u_{\tau}^2 = \frac{0.3164U_{\text{mean}}^2}{8Re^n}.$$
(19)

Substituting into Eq. (16) yields

$$\tau_p^+ = \frac{0.3164}{8} Stk \ Re^{1-n}.$$
(20)

Eq. (20) gives the non-dimensional relaxation time in terms of Stokes and Reynolds numbers, showing the dependence of deposition on these two parameters. Unfortunately, this is only valid for fully developed, smooth, turbulent pipe flow. A similar expression for the mouth and throat cannot be derived analytically as there is no such simple relation for u_{τ} , partly because it is inhomogeneous due to the complexity of the geometry and partly because of the transitional nature of the flow. However, it explains the Reynolds number dependence of deposition due to the turbulent nature of the flow. Other flow characteristics, such as the extent of separated regions and jettal flow structures could also be contributing to the Reynolds number effect on deposition. This affirms the importance of an accurate representation of the flow field and the value in performing DNS which captures all the scales in the flow.

The empirical correlation of Grgic et al. (2004b), *Stk Re*^{0.37}, suggests that the ratio of friction velocity to mean velocity decays faster with Reynolds number in the mouth and throat, $(u_{\tau}/U)^2 \propto Re^{-0.63}$, than it does in a pipe, $(u_{\tau}/U)^2 \propto Re^{-0.25}$. The derivation of the latter has herein assumed an expression for the friction factor (Eq. (18)) which applies only in fully turbulent pipe flow conditions. It is therefore expected to differ from the flow in the extrathoracic airways which is spatially developing, transitional, and includes features such as separation and impinging jets.

5. Summary

The work presented herein is the first set of direct numerical simulations of the flow in realistic extrathoracic airways, and the first numerical study of the effect of geometric variation on the flow. The results demonstrate that the flow in the extrathoracic airways is complex due to their geometry, which varies significantly across subjects. For a given flow rate, this geometric variation leads to different Reynolds numbers, which results in different flows and leads in turn to different

deposition patterns. Variation is observed even within the same subject, where the position of the tongue can create significant geometric differences resulting in qualitatively different flow features. For example, the impinging pharyngeal jet present in geometry S1b does not exist in S1a, where the tongue is pulled back. This variation is even more pronounced across subjects, as is observed by comparison of geometries S2 and S4 with S1a and S1b. Differences in the mean flow (impinging jets, separated shear layers, vortical patterns) as well as in the velocity fluctuations can be observed, both of which have an effect on particle trajectories and deposition.

The dependence of deposition on the Reynolds number, observed in the *in vitro* experiments conducted by Grgic et al. (2004b), is due to the difference in the mean flow field as well as the difference in the turbulence intensities. The better collapse of deposition data observed in the literature, when plotted against the empirical correlation *Stk Re*^{0.37} rather than *Stk* alone, is due to the fact that the Stokes number fails to account for the level of turbulence intensity in the airways. Therefore, it only takes into account impaction as a deposition mechanism, and does not include the turbulent dispersion experienced by the aerosol particles due to velocity fluctuations. By use of the dimensionless particle relaxation time, τ_p^+ , which takes into account both these deposition mechanisms, the origin of this Reynolds number dependence was explained.

Although the Reynolds number correction improves the collapse of deposition data, scatter is still observed in the literature. An explanation is provided by considering intersubject variation of the flow field. Even at the same Reynolds number and flow rate, as is the case in geometries S2 and S4, flow features can differ significantly due to geometric variation. Therefore, plotting deposition against Stokes and Reynolds numbers based on mean length and velocity scales does not entirely eliminate scatter, since the diameters of the geometries, and hence the velocities, deviate considerably from the mean in many sections of the airways. The question of appropriate scaling for flow in the extrathoracic airways has been a point of discussion in the literature (Ball et al., 2008) and remains a challenge in providing an accurate model of extrathoracic deposition, which reinforces the importance of efficient subject-specific prediction.

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