NUMERICAL STUDY OF PARTICLE DEPOSITION IN THE HUMAN UPPER AIRWAYS WITH EMPHASIS ON HOT SPOT FORMATION AND COMPARISON OF LES AND RANS MODELS

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Abstract.

A CT based simplified upper human airway model was created by preserving all critical geometrical features. The fluid flow at breathing flow rates of 30 L/min and 60 L/min are numerically studied employing RANS and LES methodology. The deposition efficiency and the deposition patterns for the particle diameters 2, 4, 6, 8 and 10 μ m are presented. In this paper special emphasis is given to the identification of possible hot spots of particle accumulation. Such spots might be responsible for the development of cancerous lesions. For smaller particle size (2 μ m and 4 μ m) RANS shows accumulations of particles (or hot spots) at epiglottis and just above glottis while LES shows negligible amount of particle accumulation. For bigger sized paticles (8 μ m and 10 μ m) the locations of the hot spots remain essentially the same in mouth and pharynx regions. The only difference between RANS and LES is that, RANS predicts a hot spot at the mouth roof while LES doesn't.

1 INTRODUCTION

There are two aspects of conducting a numerical study of particle deposition in human upper airway also called extra-thoracic region : 1) Devising an effective aerosolized medication for curing many respiratory problems, 2) To identify possible hot spots of particle accumulation which can lead to adverse health effects such as cellular-damage, inflammation and tumor formation. In the present study a CT based simplified upper human airway was created by preserving all critical geometrical features [1]. The complex extra-thoracic airway geometry act as an effective filter which limits the amount of inhaled aerosols that enter the lungs [2] due to deposition and clearance in the oral airway [3, 4]. The transport and deposition of micro-aerosols in the oral airway present a significant health risk considering that these particles carry a large dose, have a high probability for impaction and may generate large local regions of enhanced particle deposition, referred to as hot spots [5].

The flow field pattern and the properties of the inhaled particles affect the aerosol deposition in the airway [2]. The mechanisms of the airway particle deposition can be separated into two parts: the flow field generated by the airway geometry, and the interaction of aerosol particles with this flow field [6].

Experimental studies have been carried out by many authors to study the flow field and particle deposition using in-vivo and in-virto techniques. For instance Johnstone et al. [6] using hot wire anemometry observed that the basic flow features during steady inspiration include flow separation from a curved backward facing step (the teeth), flow expansion in the oral cavity downstream from the teeth, a rapid curvature of the cavity with attendant Dean-like secondary flow generation followed by flow acceleration at the back of the throat. The fluid then passes over another backward facing step (the uvula) and the epiglottis region where it is expected that large pressure gradients alter the flow as it negotiates the tortuous path past the larynx and into the pipe that is the trachea. Grgic et al. [7] reported the regional and the total deposition efficiency based on seven geometries using gamma scintigraphy and gravimetric methodology. Hennan et al. [8] performed a PIV measurement in the central sagittal plane of two realistic extra-thoracic airway geometries. They reported that there is a strong connection between local particle deposition and the local fluid velocity.

In the past many authors have conducted numerical studies to predict fluid flow field and particle deposition using RANS models. Previously many authors like Katz et al. [9], Stapleton et. al [10] used, k- ε turbulence model but failed to predict accurately the flow dynamics and the aerosol deposition. Zhang and Kleinstreuer [11] showed that LRN k- ω turbulence model can accurately predict fully laminar regions and also can predict transitional regions in a 3D conduit. Similarly Matida et. al [12] observed better results while using k- ω turbulence model as compared to using k- ε turbulence model. Though LRN k- ω turbulence model was able to predict transitional regimes yet when the percentage aerosol deposition for particles with low Stokes numbers was compared with the experimental results they found RANS model to greatly over predict the percentage deposition.

Due to morphological complexity of the extra-thoracic region a realistic mouththroat model based study is not feasible as it is time consuming and costly from both numerical and experimental point of view. Thus using a CT based simplified upper human airway model seems logical.

2 NUMERICAL METHODS

The fluid and particle phase were solved employing the incompressible solver of FLUENT 6.3

2.1 Fluid Phase

RANS: The time-averaged Navier–Stokes equations are modeled employing low Reynolds number variant of SST k- ω model (Menter [13]), which requires resolving the near-wall region with a fine mesh. This model has been selected based on its ability to accurately predict the particle depositions in the models of mouth–throat geometries [12, 14, and 15]. Second-order upwind scheme for momentum equation and third-order MUSCL scheme for k- ω equation were employed for spatial discretization. SIMPLE algorithm was used for pressure–velocity coupling.

LES: In LES, the big three-dimensional eddies which are dictated by the geometry and boundary conditions of the flow involved are directly resolved, whereas the small eddies which tend to be more isotropic and less dependent on the geometry are modeled. In the present work wall adapting local eddy viscosity model was used (WALE model) [16].

The sub-grid-scale stresses (τ_{ij}) resulting from the filtering operation is given by

$$\tau_{ij} - \frac{1}{3}\tau_{kk} = -2\mu_t S_{ij} \tag{1}$$

Where μ_t is the turbulent viscosity, S_{ij} is the rate of strain rate tensor. In WALE model, the eddy viscosity is modeled by using Eq. 2

$$\mu_{t} = \frac{\rho L_{s}^{2} \left(S_{ij}^{d} S_{ij}^{d} \right)^{3/2}}{\left\{ \left(\overline{S_{ij}} \ \overline{S_{ij}} \right)^{3/2} + \left(S_{ij}^{d} S_{ij}^{d} \right)^{5/4} \right\}}$$
(2)

where L_s is the mixing length for the sub-grid scale given by $min(\kappa d, C_{\omega}V^{1/3})$. κ is the von-Karman constant, d is the distance to the closet wall and C_{ω} is taken to be 0.325. V is the computational cell volume. Second-order implicit formulation is used for temporal discretization and central differencing for spatial discretization of momentum equation.

2.2 Particle phase

Assuming large particle-to-air density ratio, negligible particle rotation, no interparticle collision, and drag force as the dominant point force, the Lagrangian equations governing the particle motion are given by:

$$\frac{dx_p}{dt} = u_p \tag{3}$$

$$\frac{du_p}{dt} = F_d \left(u - u_p \right) + \frac{g_x \left(\rho - \rho_p \right)}{\rho_p} \tag{4}$$

Where x_p is the particle position. ρ and ρ_p are the fluid density and the particle density, respectively. g_x is the st the gravitational force which is oriented in the vertical direction.

The unbalanced pressure distribution on the surface of the particle due to the difference in fluid velocity u and particle velocity u_p is termed as the drag force F_d which is given by

$$F_d = \left(\frac{18\mu}{\rho_p d_p^2}\right) \left(\frac{C_d R_e}{24}\right) \tag{5}$$

 μ is the dynamic viscosity of the fluid. d_p is the diameter of the particle. C_d is the coefficient of drag given by:

$$C_d = a_1 + \frac{a_2}{R_e} + \frac{a_2}{R_e} \tag{6}$$

The a_i coefficients are constants for smooth spherical particles as given by Morsi and Alexander [17]. R_e is the particle Reynolds number defined as:

$$\frac{\rho d_p |u - u_p|}{\mu} \tag{7}$$

RANS:

The instantaneous velocity (u) comprises of a mean component (\bar{u}) and a fluctuating component (u'). Assuming isotropic turbulence, the fluctuating component is expressed as [18].

$$u' = \sqrt{\frac{2}{3}k} \zeta \tag{8}$$

where k is the turbulent kinetic energy of the flow and ζ is a random number drawn from a Gaussian probability density function with zero mean and unit standard deviation. The chosen fluctuation is referred to a turbulent eddy whose time scale is given by:

$$T_e = 2T_L \tag{9}$$

$$T_L = C_L \frac{1}{\omega} \tag{10}$$

 T_L is the Lagrangian time scale and the constant C_L for the SST k- ω turbulence model is 0.15. It is accepted that the fluctuation remains constant within a turbulent eddy during its life-time (T_e), while the respective mean velocity component (\bar{u}) is varied according to particle position. The crossing trajectory effect is taken into account by limiting the crossing time to

$$t_{cross} = -\tau \ln\left[1 - \left(\frac{L_e}{\tau |u - u_p|}\right)\right] \tag{11}$$

where τ is the relaxation time of the particle

LES:

In the unsteady mode, each fluid phase iteration is followed by particle phase iteration and the particles are tracked in the real time. Hence, the effect of resolved large-scale instantaneous velocity on the particles is accounted for. It is assumed that the effect of the unresolved fluctuations is negligible so that there is no need for an eddy interaction type model as in RANS.

3 RESULTS.

3.1 Fluid Phase

Figure 1 shows the time averaged velocity magnitude and stream lines at central sagittal plane for LES at 30 L/min. The flow entering through the mouth piece impinges on the tongue and takes a bend upwards. As it continues to move forward, it accelerates in the middle part of the mouth due to reduction in cross-sectional area. At the end of mouth region, the flow takes a downward turn and enters the pharynx in the form of a jet which undergoes an expansion due to increase in cross-sectional area. Consequently, the velocity is reduced and complex secondary motions are set. Just beyond the epiglottis region, the flow again accelerates due to the reduction in cross-sectional area and a clear high velocity zone develops on the posterior side of sections C1–C2. At the end of the pharynx, a step on the posterior side guides the flow towards the anterior side of the trachea in the form of a laryngeal jet. As a result of this laryngeal jet, two distinct recirculation zones originate at the posterior side at sections F1–F2.

To gain insight in to the flow physics as predicted by RANS and by LES, nondimensional velocity and turbulent kinetic energy contours at central sagittal plane are plotted and compared (see Figs. 2 and 3). In RANS the shape of the laryngeal jet is much more pronounced and longer while in LES the laryngeal jet diffuses much more rapidly. Moreover the flow physics essentially remains the same when the flow rate is increased from 30 L/min to 60 L/min. For RANS and LES the difference lies only in the respective magnitudes, this observation was also made by Kleinstreuer et. al [14].



Figure 1. The time averaged velocity magnitudes and the stream lines corresponding to central sagittal plane for 30 L/min using LES



Figure 2. Non-Dimensional Velocity contour at central sagittal plane.



Figure 3. Non-Dimensional Turbulent Kinetic energy at central sagittal plane.

Figure 4 and 5 shows the variation of velocity and turbulent kinetic energy at two crosssections. It can be observed that the velocity magnitude and kinetic energy profile obtained from RANS is very much different from LES. Fig. 4(d) and 5(d) again shows that the spread of the laryngeal jet in RANS is narrower when compared with prediction from LES.





Figure 4. Normalized Velocity Magnitude and Turbulent Kinetic energy corresponding to central sagittal plane, (a)-(d) five millimeters above epiglottis.



Figure 5. Normalized Velocity Magnitude and Turbulent Kinetic energy corresponding to central sagittal plane, (a)-(d) 1 tracheal diameter downstream of glottis.

3.2 Deposition patterns

In dilute suspensions, the main mechanisms of particle deposition are due to gravitational sedimentations and deposition due to inertial impaction. While the gravitational sedimentation depends upon the particle size, the deposition due to inertial impaction depends upon the mass of the particle (i.e. particle size and density) and the flow velocity. For gravitational sedimentation to occur, the particle residence time should be large which generally occurs in the last five to six generations of airways (smaller bronchi and bronchioles) and in the alveolated region of the lung, where the air velocity is low [19].

In order to study particle deposition, the model has been grouped into three regions namely mouth, pharynx and larynx+trachea (see Fig. 6). It can be seen from Fig. 7 and 8 that as the particle size increases the percentage deposition in the mouth region increases. In general, particle having size of 5μ m diameter is considered as the upper limit of respirable range for inhalation of drugs. The percentage deposition given by histogram shown in Fig. 9 and 10 indicates that, the small particles (2 and 4 μ m) are more able to penetrate deeper inside the lungs. Whereas particles having size 8 μ m and 10 μ m are mostly filtered out in the mouth region.

Figures 7 and 8 shows the particle deposition patterns and positions of possible hot spots for 30 L/min and 60 L/min using RANS and LES.



Figure 6. Classification of three different regions in the Simplified Human upper airway model



Figure 7. Comparision of the deposition patterns corresponding to central sagittal plane for 30 L/min for different particle diameters.



Figure 8. Comparision of the deposition patterns corresponding to central sagittal plane for 60 L/min for different particle diameters

RANS simulation indicates that the particles accumulation is large at the front of the tongue and at the mouth roof for 8 μ m and 10 μ m. The particles of size 8 μ m and 10 μ m diameter (high Stokes number) cannot follow the curved oral airway morphology and deposit due to inertial impaction. There are two hot spots locations in the pharynx region for all particle sizes. The first location is just above the epiglottis, while the second location is at the back of the pharynx. Increasing the particle size only increases the percentage deposition while the location of hot spots is the same at this region. At the larynx-trachea region, the particles accumulation is more or less distributed especially close to the glottis. This distribution is due to the complex secondary structures originated as a result of intermittent flow expansion and contraction. In this region, the particle deposition efficiency increases as the particle size increases.

In LES there is a subtle difference between the predictions of particle deposition patterns for smaller particles. LES predicts essentially negligible amount of particle deposition in mouth and pharynx region for smaller sized particles ($2 \mu m$ and $4 \mu m$). For bigger sized particles ($8 \mu m$ and $10 \mu m$) the pattern remains essentially the same as predicted by RANS the only difference was while RANS predicted the accumulation of particles at the roof of the mouth while LES doesn't. When plotted against the experimental fit given by Grgic et. al [7] (see fig. 11 and 12) it can be seen that for smaller sized particles ($2 \mu m$ and $4 \mu m$) LES gives a better prediction. For bigger sized particles ($8 \mu m$ and $10 \mu m$) the deposition efficiency essentially remains the same in RANS and LES.



Figure 9. Percentage Deposition corresponding central sagittal plane using 30 L/min



Figure 10. Percentage Deposition corresponding central sagittal plane using 60 L/min



Figure 11. Deposition efficiency for 30 L/min.



Figure 12. Deposition efficiency for 60 L/min

4. CONCLUSIONS

In the present work CT based simplified upper airway was numerical studied using RANS and LES at an inhalation rate of 30 L/min and 60 L/min. Above 5µm particle size which is generally considered an upper limit of respirable range for inhalation of drugs, both LES and RANS performs equally well. For smaller particle size (2µm and 4µm) RANS shows accumulations of particles (or hot spots) at epiglottis and just above glottis while LES shows negligible amount of particle accumulation. For bigger sized paticles (8µm and 10µm) the locations of the hot spots remain essentially the same in mouth and pharynx regions. The only difference between RANS and LES is that, RANS predictes a hot spot at the mouth roof while LES doesn't.

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