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Numerical analysis of stochastic dispersion of micro-particles in turbulent flows in a realistic model of human nasal/upper airway

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ABSTRACT

Turbulent flow field and particle deposition in a realistic model of human upper airway system including: nasal cavity, nasopharynx, oropharynx, larynx and trachea were analyzed numerically. The Lagrangian approach was used to find the trajectories of micron-size particles for the breathing rates of 30, 45 and 60 l/min. The continuous phase flow was evaluated using a RANS (Reynolds Average Navier-Stokes) turbulence model and the effect of turbulent fluctuations on particle trajectories was modeled using a continuous random walk (CRW) stochastic model, which is based on the normalized Langevin equation. The total and regional deposition fractions of micro-particles were evaluated and the effect of turbulent fluctuations on the particle deposition rate was investigated.

1. Introduction

Deposition of inhaled particles in the airway passages has been of serious health concerns. These particles include dust, microorganisms, photochemical smog and other irritants. From the toxicologic point of view, all particles which are smaller than 10 μm in diameter can be biologically active and could cause allergic responses and even cancers in susceptible individuals (Heyder, 2004; Cheng, 2003). On the other hand, for therapeutic inhalation drug delivery it is important to make sure particle deposition occurs at targeted areas. Some pharmaceutical aerosols are larger than 20 μm in order to maximize the deposition of these particles in nasal cavities and pharyngeal passage before entering the lungs. On many other cases particles smaller than 5 μm (Suman et al., 2006) and sometimes in the sub-micrometer size range are used in order to deliver the drug to the lungs (Longest & Hindle, 2010). Thus, estimating the fraction of particles that penetrates into the lung and predicting the distribution of deposited particles in different regions of the human upper airways is of considerable interest not only to determine what reaches the lung, but also to quantify the dose to upper airways for both the health risk and therapeutic effectiveness of inhaled particles.

Particle deposition in the nasal airway has been the subject of many investigations and the effect of different factors has been studied both numerically and experimentally. Although numerous experimental studies have been performed to measure total nasal deposition, both in vivo and in vitro methods have limitations. In fact, while the most physiologically

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realistic technique is utilizing human volunteers, they are limited by the number of flow rates and particle sizes that can be used and are associated with inter-subject variability. In contrast, nasal replica casts offer the opportunity to detailed measurements of the nasal passage and can be studied for a wide range of flow rates and particle sizes. There are, however, limitations on the level of surface finish in the manufacturing process which always affects airflow and the deposition of micron-sized particles or smaller (Schroeter et al., 2011).

Computational fluid dynamics (CFD) method, which gained more popularity due to the advances in computer technologies, can provide an alternative to the experimental techniques for predicting particle deposition in nasal airways. In the recent decade, the CFD approach was employed by a number of investigators (Liu et al., 2007, 2010; Shanley et al., 2008; Shi et al., 2007; Xi & Longest, 2008; Kimbell, 2006; Wang et al., 2009; Moghadas et al., 2011; Abouali et al., 2012). While most of the previous numerical works are restricted to the nasal passages from nostrils to the end of nasopharynx, some others such as the work of Martonen et al. (2002) are devoted to models which were extended to the end of trachea or first bronchial branch. Recently Farhadi Ghalati et al. (2012) developed a more comprehensive model which covers the upper airways to the end of trachea for laminar airflow regime. In the current study, this model was used and the particle trajectories under turbulent airflow regime were analyzed.

Although particles are carried by the breathing air through the respiratory system, their trajectories differ from the airflow streamlines due to their inertia and effects of various forces. The most important forces are gravity, drag, and the Brownian excitation. Particles are then deposited on the walls of the airway by sedimentation, impaction, and/or diffusion mechanisms (Heyder, 2004).

There are two methods for analyzing particle transport and deposition, namely, the Lagrangian and the Eulerian methods. The Eulerian approach is more efficient for ultra fine particles when the Brownian excitation is dominant, while the Lagrangian approach is more suitable for dilute suspension of larger particles for which the inertia is important. In this study, the Lagrangian method was used and the particles were treated as a discrete phase. For the dilute suspension the particle effects on the airflow and the particle–particle interactions are ignored. Trajectories of a large number of particles are evaluated by solving the corresponding equations of motion.

Small particles in a turbulent airflow stream are influenced by the turbulence fluctuating velocities leading to turbulence dispersion. For a reliable analysis of particle trajectories, these fluctuations should be calculated and the corresponding instantaneous flow velocity should be evaluated.

The most accurate approach for evaluating the fluctuation velocity in turbulent flows is the Direct Numerical Simulation (DNS), which is followed by the Large Eddy Simulation (LES) method. For DNS, the Navier-Stokes equation is solved using sufficiently fine grids that can resolve the Kolmogorov scale and small time steps to capture the smallest eddies and highest frequencies of turbulence. When the grid size is somewhat larger than the Kolmogorov length scales, the LES method is used, where scales larger than the grid are resolved and the effect of subgrid scale fluctuations are modeled. However, the DNS and the LES are computationally expensive. While some investigators (e.g., Dehbi, 2011; Liu et al., 2007; Liu et al., 2010) used LES in their analysis, most researchers used the Reynolds Averaged Navier-Stokes (RANS) equations and a turbulence model. In these cases the effect of turbulence subgrid scale fluctuations need to be included.

The RANS models were used by many previous investigators. For example Katz et al. (1999) and Stapleton et al. (2000) used the standard k-ε model and Renotte et al. (2000) used the RNG, k-ε model. Some researchers tried to first validate the models for similar but simpler flow fields and then apply them to more complex flows. For example, Zhang & Kleinstreuer (2003) tested different 2-equation turbulence models and recommended the use of the standard k-ω model with low-Reynolds corrections for low-Reynolds number flows which includes laminar to turbulent transition. The application of the standard k-ω model can also be found in the work of Matida et al. (2004), Grgic et al. (2006), Ball et al. (2008), Tavakoli et al. (2009), and Alexopoulos et al. (2010). The SST k-ω is another k-ω based turbulence model which was used by Liu et al. (2007, 2010) and Jayaraju et al. (2007, 2008). Earlier Li & Ahmadi (1995) used an anisotropic nonlinear turbulence model and analyzed particle deposition in the first lung bifurcation. In this study a Low Reynolds Number (LRN) k-ε model that was developed by Launder and Sharma (1974) was used.

As noted before, the RANS models compute the mean flow field. To include the turbulence dispersion effect on particle trajectories, the fluctuating velocity field at the location of particles needs to be evaluated. Typically the Discrete Random Walk (DRW) and the Continuous Random Walk (CRW) models are used.

In DRW models, which are also known as Eddy Interaction Models (EIM), it is assumed that each particle has a succession of interactions with turbulent eddies that have limited life and length scales and the fluctuating velocities can be found from turbulent quantities of the eddies. The original form of this model was proposed by Gosman & Ioannides (1983) and was used by some previous researchers such as Katz et al. (1999), Jayaraju et al. (2007, 2008), Kleinstreuer & Zhang (2003) and Liu et al. (2007, 2010) in order to take into account the turbulent fluctuations effect on particle dispersion in respiratory system. It should be noted that the use of the original DRW model for inhomogeneous and anisotropic turbulent flows can lead to unrealistic results and the particle deposition would be overestimated, since this model shows a tendency for small particles to concentrate near the walls, especially in the diffusion dominated flows (Mehel et al., 2010). In fact, when this model is combined with turbulence RANS models, it is assumed that the flow is homogenous and isotropic. One major issue with the k-ε and k-ω models is that they are based on the Boussinesq approximation which assumes the turbulence flow field to be isotropic. Therefore, the use of k-ε or k-ω models in combination with the DRW model leads to unphysical particle dispersion predictions. Also Tian & Ahmadi (2007) showed that the use of this model in combination with Reynolds Stress Models (RSM) can lead to over-prediction of particle deposition rate even in simple flows like 2D parallel duct flow.