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Particle deposition in a realistic geometry of the human conducting airways: Effects of inlet velocity profile, inhalation flowrate and electrostatic charge

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ABSTRACT

Understanding the multitude of factors that control pulmonary deposition is important in assessing the therapeutic or toxic effects of inhaled particles. The use of increasingly sophisticated in silico models has improved our overall understanding, but model realism remains elusive. In this work, we use Large Eddy Simulations (LES) to investigate the deposition of inhaled aerosol particles with diameters of $d_p = 0.1$, 0.5, 1, 2.5, 5 and 10 μm (particle density of 1200 kg/m^3). We use a reconstructed geometry of the human airways obtained via computed tomography and assess the effects of inlet flow conditions, particle size, electrostatic charge, and flowrate. While most computer simulations assume a uniform velocity at the mouth inlet, we found that using a more realistic inlet profile based on Laser Doppler Anemometry measurements resulted in enhanced deposition, mostly on the tongue. Nevertheless, flow field differences due to the inlet conditions are largely smoothed out just a short distance downstream of the mouth inlet as a result of the complex geometry. Increasing the inhalation flowrate from sedentary to activity conditions left the mean flowfield structures largely unaffected. Nevertheless, at the higher flowrates turbulent intensities persisted further downstream in the main bronchi. For $d_p > 2.5$ μm, the overall Deposition Fractions (DF) increased with flowrate due to greater inertial impaction in the oropharynx. Below $d_p = 1.0$ μm, the DF was largely independent of particle size; it also increased with flowrate, but remained significantly lower. Electrostatic charge increased the overall DF of smaller particles by as much as sevenfold, with most of the increase located in the mouth–throat. Moreover, significant enhancement in deposition was found in the left and right lung sub-regions of our reconstructed geometry. Although there was a relatively small impact of inhalation flowrate on the deposition of charged particles for sizes $d_p < 2.5$ μm, impaction prevailed over electrostatic deposition for larger particles as the flowrate was increased. Overall, we report a significant interplay between particle size, electrostatic charge, and flowrate. Our results suggest that in silico models should be customized for specific applications, ensuring all relevant physical effects are accounted for in a self-consistent fashion.

1. Introduction

Aerosol particle deposition in the airways depends on several parameters, such as the physical and hydrodynamic characteristics of the particles themselves, the inhalation flowrate, the health state of the individual and the geometrical and morphological details of the airways. A considerable amount of investigative effort in terms of experiments and numerical simulations has been directed at determining deposition efficiencies. Early studies have afforded us a satisfactory level of understanding of general trends in deposition efficiencies as a function of particles sizes. They have also improved our understanding of the airflow characteristics. For example, today we have a much better appreciation of the effects of flow turbulence in the conducting airways than we did 20 years ago (Kleinstreuer and Zhang, 2010; Lin et al., 2013). Yet, this overall understanding falls short of the precision one needs when optimizing pharmaceutical products consisting of inhaler-formulation pairs or when establishing links of particular pollutants to specific disease pathways in the airways. To complicate matters further, anatomical variations between individuals, which can be either hereditary or due to disease-induced airway remodeling, alter

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deposition to a degree that is modulated by particle size and charge, flowrate, and other factors.

In vivo studies of aerosol deposition in the human lungs are limited by concerns over human safety and by resolution limitations of current imaging technologies. In silico models based on Computational Fluid Dynamics (CFD) can fill this gap by providing an unprecedented level of detail that would allow scientists and engineers to experiment with alternate designs and conditions.

Recent studies revealed the unsteady and turbulent nature of the flow in regions downstream of the glottis, with turbulent effects dissipating only in the deeper conducting airways where the local Reynolds number decreases gradually (Kleinstreuer and Zhang, 2010; Tawhai and Lin, 2011). There are three techniques for solving turbulent flow equations using a computer: direct numerical simulations (DNS), Reynolds averaged Navier–Stokes (RANS) and large eddy simulations (LES). DNS tracks the details of the instantaneous turbulent fluctuations at all scales, however, it is exceedingly costly to implement and beyond routine use on current computers. Presently, most CFD simulations solve only for the mean flow using the RANS equations, resulting in a tremendous reduction in computational cost. However, the laminar-turbulent-laminar flow transition in the conducting airways is challenging for RANS and care must be exercised to choose validated RANS models (Xi and Longest, 2007). A more robust choice is the method of Large Eddy Simulations (LES), where the smallest scales of motion (containing a small fraction of the kinetic energy) are discarded. The computational expense of LES is considerably higher than that of RANS, but it retains significantly more elements of the underlying turbulence physics than RANS (Choi et al., 2009; Radhakrishnan and Kassinos, 2009). With constant gains in computing power, LES has become affordable for routine use and recent LES-based deposition studies have established the trustworthiness of the method.

In the case of inhaled pollutants, ambient conditions such as the air and aerosol characteristics in the breathing zone of an occupant can be expected to play a role in determining deposition in the airways. Longest et al. (2008) investigated the deposition characteristics of ambient and capillary-generated spray aerosols in a realistic mouth–throat geometry. They found that spray momentum effects induce significantly more deposition than ambient aerosols, especially in the first section of the mouth–throat geometry as a result of spray inertia interacting with the tongue. In the absence of a free stream airflow (e.g. as caused by a ventilation system), the air flowfield in the breathing zone results from the interaction between the occupant's breath with a free convection flow around the body. Temperature differences between the body surface and the surrounding air drive the free convective flow, which starts slow and laminar with a thin boundary layer at the lower parts of the body, but becomes faster and turbulent with a thick boundary layer at the height of the head (Lewis et al., 1969; Licina et al., 2014). Airborne particles close to the ground can be transported by the convective flow into the breathing zone, a process that has a potentially negative impact on the quality of the inhaled air (Licina et al., 2015a,b). Aerosols and air parcels are transported by the free convective flow with sufficient momentum and turbulence intensities to alter the characteristics of the flowfield in the pharyngeal cavities during inhalation, but these effects remain largely unexplored.

A second important determinant of deposition is the respiratory flowrate, which is crucial during the patient initiated maneuver for inhaling medicines, but also during exposure to environmental pollutants. Flowrates of 15, 30 and 60 l/min are considered to correspond to sedentary, light and heavy activity conditions (Xi and Longest, 2007), while in the cases of rapid inhalation, typically encountered during the use of pharmaceutical aerosol inhalation devices, inhalation flowrate can reach values up to 120 l/min (Johnstone et al., 2004). A higher flowrate causes earlier transition to turbulence in the upper airways and the ensuing fluctuations make aerosol particles move erratically, thus altering deposition patterns in a size-dependent fashion. Also, turbulence produced in the oropharynx can be advected to several generations of the tracheobronchial tree, as estimated in Finlay (2001), for a simplified cylinder-based airway model and for airflow Reynolds numbers above 2000 in the larynx.

Electrostatic charge carried by inhaled particles is also an important determinant of deposition, especially in the case of drug delivery. Medical devices such as nebulisers, Metered Dose Inhalers (MDI) and Dry Powder Inhalers (DPI) often generate electrostatically charged aerosols (Byron et al., 1997; Kwok et al., 2005). But even environmental aerosols may have charges well above the Boltzmann equilibrium and thus electrostatic charge must be taken into account in human health risk assessments (Forsyth et al., 1998). Several theoretical studies in lung models (Yu, 1985; Bailey et al., 1998), experiments in man (Melandri et al., 1983; Prodi and Mularoni, 1985) as well as clinical measurements confirmed that charge carried by particles enhances the deposition of the particles in the lung considerably. This is not desirable for drugs intended for systemic uptake, which must pass into circulation through the alveolar epithelium, but might be desirable for drug delivery in certain upper regions of the airway tree or even leveraged for the removal of pollutant particles using electrostatic charge effects (Ali et al., 2008).

In this work, we use LES to study the effects of the mouth inlet velocity profile and of electrostatic charge at various inhalation flowrates on particle deposition patterns inside a realistic model of the human upper airways. Specifically, two different inlet conditions are examined under steady inhalation at a flowrate of 4.5 l/min. The first is a uniform velocity profile, as used in most current computational studies. The second is a velocity profile measured by us in the breathing zone of a breathing thermal manikin using Laser Doppler Anemometry (LDA), which is closer to the real case. The experiments to generate the measured profile are beyond the scope of the present paper and will be described in a separate publication. The effect of inhalation flowrate is examined by considering flowrates of 15, 30 and 60 l/min, while assuming uniform inlet velocity. Finally, deposition enhancement in the lungs due to electrostatic effects is also assessed as a function of inhalation flowrate.

2. Methods

2.1. Airway geometry

Early in silico models relied on simplified representations of the human airways, with many of them employing the symmetric model of Weibel (1963). Recent advancements in medical imaging have afforded us detailed views of the complex structures of the lung. The geometry considered in this study, (see Fig. 1(a) and (b) – coordinate system is also shown) is reconstructed from Multi-Detector Computed Tomography (MDCT) scans and it represents a non-smoking 20 year old female. This geometry was provided to us by the Department of Mechanical and Industrial Engineering of the University of Iowa (USA) and was also used in the study of Choi et al. (2009), where more details regarding the MDCT reconstruction method and the airway dimensions can be found. The respiratory tract includes the extra-thoracic airways of the mouth, the oropharynx, the laryngopharynx, the larynx and the trachea as well as the intrathoracic airways up to generation 7. Table 1 summarizes the geometrical features of the reconstructed airways (average cross sectional area A and corresponding hydraulic diameter D_h) along with the key flow parameters (bulk velocity U and Reynolds number Re) for the three higher flowrates considered in this study.

When studying the effect of different velocity profiles imposed at the mouth inlet, the airway geometry is truncated at the end of the trachea in order to reduce the mesh size and computational cost. This simplification is based on preliminary numerical experiments that had shown that all differences in the flowfield due to inlet conditions dissipate in the upper airways and well before the flow reaches the tracheal bifurcation. Also, in order to match the velocity profile measured at the