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CFD simulation of particle deposition in a reconstructed human oral extrathoracic airway for air and helium–oxygen mixtures

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In order to compare the effects of using helium–oxygen and air in assisted breathing and inhalation therapies, flow and particle deposition results were obtained in a realistic model of human oral extrathoracic (ET) airways using computational fluid dynamics (CFD) and pressure loss measurements. As the main deposition mechanism for pharmaceutical aerosols in the ET is inertial impaction, the ET model was reconstructed from medical images to take into account the complexity of realistic morphological features. Calculations were performed with the CFD software Fluent®, and pressure losses were measured on a cast based on a stereolithographic fabrication of the model. Results show that ET pressure loss and particle deposition are lower with helium–oxygen as compared to air. Moreover, further simulations were performed with various particle sizes and inspiratory flow rates, which indicate that particle deposition in the ET depends on both the Stokes and Reynolds number.

1. Introduction

Clinical and theoretical studies document the benefits of helium–oxygen gas mixtures to improve respiratory assistance (e.g. Jaber et al., 2000, 2001) and aerosol drug delivery (review by Corcoran & Gamard, 2004). As shown by Papamoschou (1995) in a simplified theoretical model of the lungs, the respiratory benefit can be explained by the decrease in airway resistance because helium–oxygen mixtures are about three times less dense than air. Moreover, the turbulent character of helium–oxygen flows is less pronounced due to the smaller density and higher viscosity of helium–oxygen mixtures in comparison to air. These physical property differences between air and helium–oxygen mixtures also promote differences in particle deposition mechanisms, which will be addressed in this paper.

As a gateway to the successive generations of the respiratory tract, the oral extrathoracic (ET) region influences entrance flow conditions and aerosol deposition in the lung. Deposition in the oral ET region is normally an undesirable effect which limits the amount of drug transmitted to the lung. As micron-sized aerosol particles reach high speeds and experience rapid changes in trajectory, they are mainly deposited by inertial impaction (Martonen, 1993). Hence, morphological details strongly affect particle deposition and, if one wants to evaluate the difference between air and helium–oxygen in terms of flow and aerosol drug delivery in the oral ET airways, it is important to consider realistic oral ET

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geometries, e.g. those obtained from medical images. In such complex geometries, flow calculations are made by computational fluid dynamics (CFD) methods or using in vitro experiments. Several studies on aerosol deposition in the oral ET region have been performed. Stapleton, Guentsch, Hoskinson, and Finlay (2000), Matida, Finlay, Lange, and Grgic (2004), Zhang and Kleinstreuer (2003), Zhang, Kleinstreuer, Kim, and Cheng (2004) worked on simplified oral ET models to improve the CFD techniques for calculation of flow and particle deposition. Matida, Finlay, Breuer, and Lange (2006) applied the large eddy simulation (LES) turbulence model in an idealized ET model and found a good comparison with experimental measurements. Jayaraju, Brouns, Verbanck, and Lacor (2007) and Ma and Lutchen (2009) used a realistic ET morphology to study deposition of particles carried by air. Xi and Longest (2007, 2008) studied the effects of the ET morphology on the deposition of micron- and nano-sized inhaled particles by comparing numerical deposition results calculated on models with different degrees of realism. These studies reveal a significant dependence of flow structures and micron-size aerosol dynamics on morphological features. Grgic, Finlay, Burnell, and Heenan (2004) performed in vitro particle depositions measurements in several ET morphologies with air and found important differences, not only between different subjects, but also between two morphological configurations from the same subject. These authors proposed to correlate and predict ET deposition based on both the Stokes and the Reynolds numbers. Finally, CFD methods were used by Gemci, Shortall, Allen, Corcoran, and Chigier (2003) to compare aerosol drug delivery with helium–oxygen and air in a throat model, but neither the mouth nor the epiglottal constriction were incorporated into the model.

This paper describes the CFD analysis of flow and particle deposition in a realistic human oral ET model reconstructed from medical data for flows of air and helium (78%)–oxygen (22%) mixture, as well as pressure loss measurements in a cast of the same morphology. The deposition results are compared with the correlation found by Grgic et al. (2004).

2. Materials and methods

2.1. Oral ET model

The oral ET region consists of the mouth, the oropharynx and the larynx. For orally inspired gas, it is the gateway to the tracheobronchial region (TB) (the nonalveolated conducting zone) and finally the pulmonary region (P) (the transitional and respiratory zone) (Martonen, 1993).

A model of the oral ET region (cf. Fig. 1) was reconstructed from two sets of medical data: the mouth was obtained from a dental impression performed on a healthy adult male and the oropharyngeal and laryngeal parts were defined from the segmentation of DICOM images acquired from high-resolution CT-scans of another living healthy adult male (Sandeau, Apiou-Sbirlea, Fodil, Isabey, & Caillibotte, 2007). The size of the mouth was slightly increased and oriented to match the oropharyngeal connection obtained from the CT-scans. The software packages Amira® (Mercury Computer Systems, Inc.) and TGrid® (ANSYS, Inc.) were used to merge the morphologies and to segment and construct the surface mesh of the model, respectively. The 3D-reconstructed surface allowed for the definition of a volumetric CFD mesh for flow calculations and the construction of a material cast in epoxy resin by stereolithography with the addition of inlet and outlet adaptors designed for experimental work. The principal geometric characteristics of the model, as defined by Longest, Hindle, and Das Choudhuri (2009), are a hydraulic diameter at the mouth opening of 1.6 cm, a glottis cross-sectional area of 1.90 cm^2, a minimum hydraulic diameter of 1.17 cm (near the top of the epiglottis) and a cross-sectional area at the trachea of 1.80 cm^2.

2.2. Flow and deposition characterization

We define in this section the Reynolds number, Re, the turbulence intensity, I_t, and the Stokes number, Stk, which are dimensionless numbers characteristic of the flow regime, the turbulence, and inertial impaction, respectively.

2.2.1. Flow regime characterization

Low values of the Reynolds number, Re, are associated with laminar flows whereas high values are associated with turbulent flows. The Reynolds number is defined as

$$Re = \frac{\rho_g U D}{\mu_g} \tag{1}$$

where ρ_g ($kg\,m^{-3}$) is the gas density, μ_g ($kg\,m^{-1}\,s^{-1}$) is the gas viscosity, U ($m\,s^{-1}$) is a characteristic flow velocity and D (m) is a characteristic length scale. As proposed by Grgic et al. (2004), U and D were calculated from geometrical characteristics of the oral ET model:

$$U = \frac{QL}{V} \tag{2}$$

$$D = 2\sqrt{\frac{V}{\pi L}} \tag{3}$$