Journal of Aerosol Science xxx (xxxx) xxx–xxx

Contents lists available at ScienceDirect

Journal of Aerosol Science

journal homepage: www.elsevier.com/locate/jaerosci

Flow features and micro-particle deposition in a human respiratory system during sniffing

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ARTICLE INFO

Keywords:
Respiratory tract
Particle transport/deposition
Computational fluid-particle dynamics

ABSTRACT

As we inhale, the air drawn through our nose undergoes successive accelerations and decelerations as it is turned, split and recombined before splitting again at the end of the trachea as it enters the bronchi. Fully describing the dynamic behaviour of the airflow and how it transports inhaled particles poses a severe challenge to computational simulations. In this paper we explore two aspects: the dynamic behaviour of airflow during a rapid inhalation (or sniff) and the transport of inhaled aerosols. The development of flow unsteadiness from a laminar state at entry to the nose through to the turbulent character of tracheal flow is resolved using accurate numerical models with high performance computing-based large scale simulations. Combining the flow solution with a Lagrangian computation reveals the effects of flow behaviour and airway geometry on the deposition of inhaled microparticles. Improved modelling of airflow and delivery of therapeutic aerosols could be applied to improve diagnosis and treatment.

1. Introduction

The sniff, a rapid and short inhalation is probably the most complex case to breathing to simulate. It involves different flow features and regimes simultaneously along the respiratory tract. The resulting airflow is composed of laminar, transitional and turbulent regimes in different airway segments. The geometry of the respiratory tract is composed of tiny passages, constriction zones and rapid changes in direction. Doorly, Taylor, Gambaruto, Schroter, and Tolley (2008) investigated variations in the nasal airways and the modelling of flow in this complex geometry, providing comparisons with numerical and experimental models (Doorly, Taylor, & Schroter, 2008). Taylor, Doorly, and Schroter (2010) demonstrated that incorporating the external nose and face reproduces the external physiological boundary conditions. Other works, such as Jayaraju, Brouns, Lacor, Belkassem, and Verbanck (2008) and Ball, Uddin, and Pollard (2008), used the human upper airway with an idealized geometry and presented results concerning mean flow and flow structures. Contrary to Jayaraju et al. (2008) and Ball et al. (2008), Ghahramani, Abouali, Emdad, and Ahmadi (2014) and Bates et al. (2017a, 2017b) used a realistic model to perform a numerical analysis in the upper human airway. Saksono, Nithiarasu, Sazonov, and Yeo (2011) and Lin, Tawhai, McLennan, and Hoffman (2007) demonstrated that incorporating the nasal cavity into the upper airway is essential in order to study the flow in the throat, since the results with and without the nasal cavity are dramatically different.

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https://doi.org/10.1016/j.jaerosci.2018.05.008
Received 1 February 2018; Received in revised form 16 May 2018; Accepted 18 May 2018

The nasal cavity is the first line of defense in the respiratory tract that filters out inhaled airborne particulate matters, thus protecting the delicate lower airways (Balásházy, Hofmann, & Heistracher, 2003). Particle deposition in human nasal cavities has been extensively studied in the past (Calmet et al., 2018; Cheng, 2003; Cheng et al., 2001, Cheng, Cheng, Yeh, and Swift, 1995; Kesavanathan and Swift, 1998; Kesavanathan, Bascom, and Swift, 1998; Kesavan, Bascom, Laube, & Swift, 2000) including nano and micro-particles, using in-vitro and in-vivo methods. However particle deposition studies based on realistic human upper airway models are less popular (Ghalati et al., 2012; Jayaraju et al., 2008). Furthermore, steady (time-constant) inhalation flow rates have also been extensively studied (Kolanjiyil & Kleinstreuer, 2013; Shi, Kleinstreuer, & Zhang, 2008b, 2007a; Zhang & Kleinstreuer, 2011). Although fewer investigations exist with unsteady inhalation flow rates, such as Bahmanzadeh, Abouali, and Ahmadi (2016) who compared micro-particle deposition under cyclic inspiratory flow with equivalent steady conditions. They concluded that while the general trend was similar, the particle deposition for equivalent steady inhalation conditions cannot accurately predict the particle deposition for cyclic inspiratory flow. To study aerosol drug delivery, unsteady particle tracking through transient (time-varying) airflow needs to be addressed in detail.

Drug delivery to the olfactory region is particularly important. This region (upper meatus below the cribiform plate) (Zhao, Scherer, Hajiloo, & Dalton, 2004) is the target of drug delivery of aerosols in the nasal cavity. The route taken by inhaled particles to reach the brain, via the olfactory pathway, is unclear. There is increasing evidence that inhaled particulate matter depositing in the olfactory region can migrate to the brain along the olfactory bulb Garcia, Schroeter, and Kimbell (2015). Due to the protected area of the human olfactory epithelium, it is estimated that only 10% of inhaled air actually reaches the olfactory region during a normal resting breath, see Hahn, Scherer, and Mozell (1993). As far as the authors know, there is no literature about micro-particle deposition in the human upper airways during sniffing.

This study aims to provide the basic information necessary to understand the flow features and the micro-particle deposition pattern happening in the human respiratory tract during sniffing. The results are presented as a journey through the human airway.

Previous studies have analyzed different aspects of the airflow with the same anatomy and boundary conditions used in this study (Bates et al., 2015; Calmet et al., 2016).

This paper is organized as follows: Section 2 presents the methods used, Section 3 presents the results of the simulation, whilst the conclusion and the discussion are presented in Section 4.

2. Methods

2.1. Geometry and mesh description

The computational domain was reconstructed from a clinically acquired computed tomography (CT) scan of a 48-year-old male subject. A consultant radiologist reported the nasal airways as clear and of normal appearance. The position of the tongue base and other soft tissues in the pharynx were deemed consistent with the patient being scanned in the supine position. The airway in the pharynx may be narrower than if the patient had been standing, but the geometry is within the normal range. Further details of the medical case are provided by Bates et al. (2015).

The surface definition was produced by semi-automatic segmentation of the medical images. This surface was then smoothed using Taubin's smoothing algorithm Taubin (1995). Further details of the segmentation are provided by Calmet et al. (2016).

An unstructured mesh was employed, due to the complex shape of the geometry, especially apparent within the intricate passageways of the nasal cavity. The mesh generation software employed was ANSYS ICEM CFD (ANSYS Inc., USA). All the meshes in this study were hybrid, made of tetrahedrons, with prism layers at the wall to resolve the boundary layer.

Three meshes were used in this study. A coarse one with 9 million elements, a fine one with 44 million elements and a very fine one with 350 million elements, see Fig. 1. In this study, particle deposition is computed only in the coarse mesh due to a relatively inefficient load balance scheme and the computational cost. We left for a future paper the required improvements to simulate particle deposition in very large meshes.

The mesh convergence study was presented previously, all the details concerning meshes and parameters are provided by Calmet et al. (2016).

2.2. Governing equation and boundary conditions

2.2.1. Fluid solver

In this section, we briefly describe the numerical method used to solve the Navier-Stokes equations: the high performance computational mechanics code Alya (Vázquez et al., 2016), which was developed at Barcelona Supercomputing Center. A deeper description of this numerical method can be found in Houzeaux and Vázquez (2008). Let μ be the viscosity of the fluid, and ρ its constant density. The problem is stated as follows: find the velocity $\boldsymbol{u}$ and mechanical pressure p in a domain Ω such that they satisfy in a time interval

$$\rho\frac{\partial \boldsymbol{u}}{\partial t} + \rho(\boldsymbol{u}\cdot\nabla)\boldsymbol{u} - \nabla\cdot[2\mu\varepsilon(\boldsymbol{u})] + \nabla p = \boldsymbol{0}, \tag{1}$$

$$\nabla\cdot\boldsymbol{u} = 0, \tag{2}$$

together with initial and boundary conditions. The velocity strain rate is $\varepsilon(\boldsymbol{u}) = \frac{1}{2}(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^t)$.