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Phase change and deposition of inhaled droplets in the human nasal cavity under cyclic inspiratory airflow

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ABSTRACT

In many situations, inhaled droplets experience phase change in the human nasal passages during the breathing cycle. The associated size change of droplets can significantly influence the transport and deposition patterns in the nasal cavity. In this study, the transport, evaporation, and deposition of inhaled droplets under unsteady cyclic breathing conditions were simulated. A computational model of the nasal cavity was developed from magnetic resonance imaging (MRI) scans of the nose of a healthy male and a computational fluid dynamics (CFD) method was used to solve the governing equations of airflow and droplet motion. The Lagrangian trajectory approach was then used to investigate the transport and deposition of droplets. The size change of droplets was simulated using a convection–diffusion controlled model. In order to evaluate the effects of evaporation on transport and deposition of droplets, two inhaled compounds (water and linalool) with different saturation vapor pressures were simulated. The results showed substantial differences between the evaporation behavior of water and linalool droplets. Water droplets, which is more volatile than linalool drops, with the initial diameter ≤ 8 μm completely evaporated while complete evaporation of linalool droplets was observed for the initial diameter < 2 μm. During the time-varying inspiratory airflow, the minimum evaporation rates were observed when the airflow rate was near its maximum value. Comparing the deposition fractions of water droplets in the presence and absence of evaporation showed that droplet evaporation decreases the deposition of droplets by about 10–20% mainly due to the reduced inertial impaction effects. Furthermore, it was shown that a steady airflow simulation does not accurately estimate the deposition and evaporation of droplets in the human nasal cavity.

1. Introduction

The nasal airway is the primary entrance of the human respiratory system and is the first line of defense against inhaling particulate matters. Before inhaled air enters the lower airways, the nasal passages filter particles larger than about 5 μm from the air. Accurate estimate of transport and deposition of inhaled particles in the nasal cavity is important not only to ascertain the amount that could deposit in the lung airways, but also to quantify the dose in the nasal passages for human health risk assessments and drug delivery purposes. Many experimental studies have been performed to measure deposition of solid particles in the human nasal passages. These experimental studies have included both *in vivo* studies using human volunteers (Heyder & Rudolf, 1975; Hounam, Black, & Walsh, 1971; Pattle, 1961) and *in vitro* studies using nasal airway replicas (Cheng, Yamada, Yeh, & Swift, 1988; Garcia, Tewksbury, Wong, & Kimbell, 2009; Kelly, Asgharian, Kimbell, & Wong, 2004a; Liu, Matida, & Johnson, 2010; Zwartz & Guilmette,

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2001). Experimental studies have shown that the aerodynamic particle diameter, the flow pattern during inhalation, and the respiratory tract geometry significantly affect the particle deposition efficiency in the human nasal cavity. In addition, these experiments suggest that the deposition of micro-particles in the human nasal passages is mainly due to the particle inertia.

An alternative to experimental methods for predicting transport and deposition of particles in the human nasal airway is using the computational fluid dynamics (CFD) approach. Because of non-invasive feature of CFD methods, they have been used widely for engineering and medical purposes. A number of CFD studies using models reconstructed from computed tomography (CT) or magnetic resonance imaging (MRI) scans have been conducted to investigate deposition of particles in the human nasal passages (Ghalati et al., 2012; Liu, Matida, Gu, & Johnson, 2007; Shanley, Zamankhan, Ahmadi, Hopke, & Cheng, 2008; Wang, Inthavong, Wen, Tu, & Xue, 2009; Xi & Longest, 2008). All of these numerical studies evaluated the transport and deposition of particles with fixed sizes (that is, their sizes were not changed as they travel through the nasal airway).

In many situations, solid and liquid inhaled particles experience size changes when traveling in the human respiratory tract. Hygroscopic particles that absorb moisture from the humid atmosphere due to condensation increase in size. A number of numerical studies have investigated the effects of condensational growth on particle size and deposition patterns in the respiratory tract of humans (Ferron, Oberdörster, & Henneberg, 1989; Kim, Xi, & Si, 2013; Longest, Tian, & Hindle, 2011; Xi, Kim, Si, & Zhou, 2013). The hygroscopic growth and deposition of cigarette smoke in the respiratory tract have also been simulated by Longest and Xi (2008) and Robinson and Yu (2001). These studies showed that hygroscopic growth under relatively high humidity conditions could significantly increase the particle size and affect the deposition patterns in the respiratory tract. For example, Ferron et al. (1989) showed that hygroscopic growth increases the deposition of particles with initial diameters between 0.5 and 2 μm by a factor of two in the human respiratory tract.

Volatile droplets, unlike hygroscopic particles, lose mass from their surfaces due to evaporation and decrease in size. Deposition and evaporation of inhaled volatile droplets in the human respiratory tract have been investigated in a number of studies. Zhang, Kleinstreuer, Kim, and Cheng (2004) simulated the motion and evaporation of fuel droplets in the oral airway and the first four generations of the tracheobronchial tree. Their results showed that evaporation of droplets significantly affects the deposition pattern in the human respiratory tract. They also demonstrated that deposition fraction of droplets due to evaporation decreases with the human inspiratory flow rate. Longest and Kleinstreuer (2005) evaluated the performance of several evaporation models to simulate evaporation of multicomponent droplets in the human upper respiratory tract. Zhang, Kleinstreuer, and Kim (2006) studied the hygroscopic and evaporative effects on deposition of saline droplets under steady-state inspiratory flow in the human upper airways. Schroeter et al. (2016) investigated deposition and phase change of semi-volatile droplets in the human nasal cavity under steady-state inspiratory flow.

Most of the earlier studies applied a steady breathing airflow assumption to solve the flow field equations in the human airway in order to decrease the computational cost and time; however, in real situations, the flow rate entering the nasal airway changes during the human respiratory cycle. A limited number of studies have been conducted to investigate the unsteady airflow in the human respiratory tract. Shi, Kleinstreuer, and Zhang (2006) showed that steady airflow assumption in the human nasal cavity could be appropriate only for $Wo \leq 4.3$ and $St \leq 0.2$, where Wo and St are Womersley and Strouhal numbers, respectively. Hörschler, Schröder, and Meinke (2010) found that steady assumption for inspiratory airflow could be used for Reynolds number greater than 1500 when St is 0.791. Transport and deposition of mono size particles in the respiratory tract have been also studied under the unsteady inspiratory airflow. Zhang, Kleinstreuer, and Kim (2002) and Grgic, Martin, and Finlay (2006) observed that the deposition of micro particles under cyclic inspiratory airflow is higher than that estimated by the steady flow simulation at the equivalent mean flow rate. Bahmanzadeh, Abouali, and Ahmadi (2016) also performed an unsteady simulation and indicated that the steady inspiratory airflow simulation with an equivalent mean flow rate is not able to evaluate the particle deposition for cyclic breathing reasonable accuracy, especially for 1–5 μm particles.

In this study, using the cyclic inspiratory airflow and accounting for the phase change and its related particle size changes, deposition of micron-sized inhaled droplets in the human nasal cavity was investigated. During the inhalation, the evaporation and deposition of droplets at different time intervals were analyzed, and effects of time-varying inspiratory airflow on behavior of droplets in the human nasal cavity were investigated. Furthermore, since most of the earlier studies used a steady airflow assumption in the airway, the effects of such an assumption on the particles behavior in the nasal cavity were also evaluated. Two different droplets (water and linalool) that are widely used in consumer products and industry were studied. The physical properties of these liquids are listed in Table 1. These liquids that have markedly different vapor pressures are suitable for assessing the effects of evaporation on transport and deposition of droplets.

2. Numerical methods

2.1. Computational model of the nasal airway

A three-dimensional CFD model of the human nasal airway was used to simulate the inspiratory airflow, phase change dynamics, and deposition of droplets (see Fig. 1(a)). The nasal airflow geometry was developed from magnetic resonance imaging (MRI) scans of the nose of a healthy, nonsmoking, 53-year-old Caucasian male (73 kg mass, 173 cm height) (Guilmette, Cheng, Yeh, & Swift, 1994; Subramaniam, Richardson, Morgan, Kimbell, & Guilmette, 1998) using a commercial software. The MRI scans consisted of 67 coronal images of the nasal passages at intervals of 1.5 mm from the tip of the nostrils to the nasopharynx. The same MRI data set has been used in multiple *in vitro* (Garcia et al., 2009; Guilmette et al., 1994; Kelly et al., 2004a; Kelly, Asgharian, Kimbell, & Wong, 2004b) and *in silico* (Schroeter, Kimbell, & Asgharian, 2006; Shi et al., 2006; Shi, Kleinstreuer, & Zhang, 2008; Subramaniam et al., 1998)

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