RESEARCH ARTICLE

Heat and mass transfer simulation of the human airway for nano-particle water vapor

Knowledge regarding the particle deposition processes in lung airway is an important issue for aerosol therapy and inhalation toxicology applications. Many researches often calculated the deposition fraction in the upper airway, but they do not frequently investigate the Nusselt and Sherwood number for inhalation. This study focuses on evaluating the injury taking place in the upper human respiratory tract, based on level of exposure to hot gases. This study uses the Nusselt and Sherwood number to evaluate the heat and mass transfers in inhalation. To this end, we reconstructed a two-dimensional model of upper airway from the mouth to trachea and used the low-Reynolds-number (LRN) k–ω turbulence equation to simulate the heat and mass transfers. The finite element method is used to solve the low-Reynolds-number (LRN) k–ω turbulence equation. The model developed for the simultaneous mouth breathing during the inspiration phase with volumetric flow rates of 10 and 50 L/min. The results of simulation show that the Nusselt and Sherwood number in inhalation increases with increasing the Reynolds number. The temperature and concentration profiles help to assess the level of damage created in the upper airway and appropriate treatment for the damage.

Q1 **By Masoud Khajenoori, Ali Haghighi Asl**

INTRODUCTION

Q2 Simulation of air–particle flow in human lung has attracted many researchers in recent years. These researchers tried to investigate the heat and mass transfer in the human respiratory tract. They demonstrated that there is a significant association between the inhalation of aerosols and increased cardiovascular and pulmonary morbidity and mortality.[1] The study of water vapor in airways can increase an understanding of the inhalation effect of harmful particles on the pulmonary drug delivery to improve the human health. The normal body temperature heats the inhale air when it passes through the upper respiratory airway. Therefore, the airway may injured if the temperature of inhale air is higher than human body.[2] The airflow velocity is usually expressed by the Navier–Stokes equations.[3] Although, a solution is presented for the Navier–Stokes equations by a complex numerical analysis, it is still widely used.

Many researchers[4,5] used a method of numerical solution for the incompressible Navier–Stokes equations. However, the solution of the Navier–Stokes equations in some specific conditions can be obtained by an analytical method.[6] Some researchers tried to expand the previous studies using the turbulent models.[7,8] They developed these models to evaluate the nano-particle profile in oral airway.[3,9] Farahmand et al. performed a three dimensional heat transfer simulation using computational fluid dynamics (CFD) software to study the temperature profile of the upper lung airway. This model consists of the nasal cavity, oral cavity, trachea, and bronchi.[10] The mathematical models of heat and mass transfer were used to determine the heat and mass transfer characteristics in the human airway regions with the numerical simulation. The nano-particles or the ultrafine particles with $d_p < 100$ nm are usually suspended in ambient air and workplace. Also, they can be generated by inhalers as drug aerosols for therapeutic purposes.[11] Yong et al. provided a transient two-dimensional mathematical model for the heat and water vapor transport across the respiratory tract. This model could predict the thermal impact of inhaled hot gas entered the nasal tissues during the early stage of fires.[12]

The aim of this paper is developed a computing model to simulate hot air flow in the lung airway which it consists of the oral cavity and trachea. This study will assist in developing safe and effective preventive measures and treatments for the injuries caused in the respiratory tract. Design of respirator devices and safety features for occupations that involve exposure to extreme and unfavorable conditions hazardous to human health can be well implemented by knowing the level of injury caused in the heat and mass transfer. The design of respirator systems used by people working in extreme environments, like firefighters

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exposed to forest fires, chemical and biological hazards, or hazardous materials, can be better improved by comprehensive study of the thermal profile. These emergency responders are exposed to extreme temperatures, and although they do have protective equipment such as respirators for oxygen supply, they still inhale air that is heated because of the extreme temperature in the surrounding atmosphere. Therefore, the transient air temperature history human airway plays an important role in the thermal injury during fires.[13] Although there have been many papers describe numerical simulation of heat and mass transfer in human airway, few efforts were ever made to profile heat and mass transfer at high temperatures in the human upper respiratory tract.[4–9] In this study, a transient theoretical model was established to describe heat and mass transfer in the human respiratory tract. The results might help us better understand the development of injury taking place in the respiratory tract exposed to various fire situations. The finite element analysis used to solve the computational model. This model could predict the heat and mass transfer of water vapor and local depositions in lung airway. The inlet temperature of the permeate nano-particle water vapor is constantly maintained at 333 K (60 °C). The reminder of this paper is structured as follows: Section "Background Information" provides the background information about two dimensional geometric model of the lung airway. Section "Governing Equations in Human Airway" describes the heat and mass transfer in human airway and the deposition of nano-particles in the 1–100 nm diameter range. Section "Nano-Particle Deposition" presents the particle deposition fractions under difference flow rate. Section "Nano-Particle Heat and Mass Transfer" presents the pressure drop across the human airway as a function of inspiratory flow rate compared with reported experimental data and the concentration and temperature profiles of water vapors in the lung airway model for different flow rate. Also, this section provides the profiles of local Nu and Sherwood number for water vapor. But, we do not find experimental data to evaluate simulation data. At Section "Conclusion" finally presents the conclusion.

METHODS

Background Information

The particle deposition in lung airway is an important factor to evaluate the efficacy of inhaled drug therapy. The detailed particle deposition characterization in the upper and lower airway using experimental techniques is expensive and difficult. Now, the numerical simulation of particle motion in airway is an effective method to tackle this problem and it can estimate the particle deposition patterns in lung airway. The lung airway is divided into the upper and lower airways. The upper airway is an important section of the lung airway that is affected by the particle deposition. Therefore, we provided a numerical simulation for the upper airway. The upper airway model consists of oral cavity (mouth and palate), pharynx, larynx and trachea. We adapt the dimensions of the upper airway model with a human cast reported by Zhang et al.[14] As shown Figure 1, the length of the mouth to the glottis and the length of the glottis to the first carina were about 12 and 14 cm, respectively.[12,14] The trachea diameter was 1.60 cm and other airway diameters were different. The airway wall in this model is assumed as smooth and rigid. We do not consider the effects of cartilaginous rings which are appeared in the upper airway. The air breathed in during the inspiration phase consists of hot nano-particle water vapor having a temperature of 60 °C. The wall is maintained at a temperature of 37 °C (the average normal temperature of the healthy human body).[10]

Governing Equations in Human Airway

There is still uncertainty on the critical Reynolds number of the flow rate for the transition of turbulent flow in the lung airway system. Moghadas et al. reported the approximation of turbulent flow for a flow rate more than 12 L/min seems reasonable especially

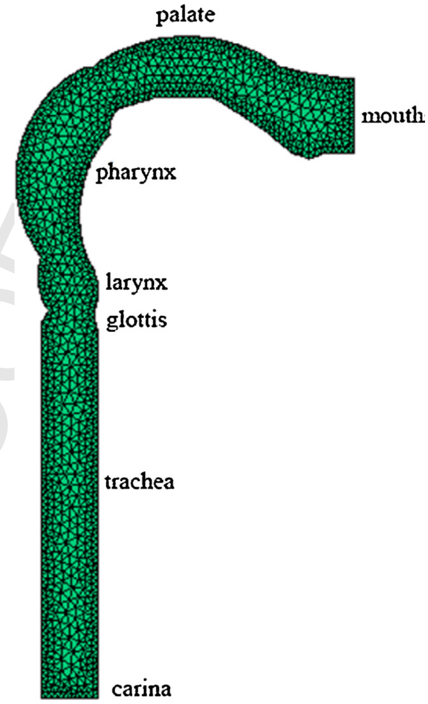

Figure 1. The 2-D upper airway model based on the model provided by Zhang et al.[3,14].

for the vibrant activities such as track and field.[15] The governing equations for the oscillating two-dimensional airflow are the Navier–Stokes equations and the continuity equation. These equations in the Cartesian coordinate can be expressed as follows[16]:

Continuity equation:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \tag{1}$$

Momentum equation:

$$\rho\left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y}\right) = -\frac{\partial p}{\partial x} + \mu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) \tag{2}$$

$$\rho\left(\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y}\right) = -\frac{\partial p}{\partial y} + \mu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) \tag{3}$$

where u and $\boldsymbol{v}$ are the components of velocity in x and y axes, respectively and p is the component of pressure. $\boldsymbol{\rho}$ and $\boldsymbol{\mu}$ are the density and dynamic viscosity of the air, respectively. The low-Reynolds-number (LRN) k–$\boldsymbol{\omega}$ turbulence equations are appropriate for

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