Computers in Biology and Medicine 74 (2016) 1–17

Contents lists available at ScienceDirect

Computers in Biology and Medicine

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

Details of regional particle deposition and airflow structures in a realistic model of human tracheobronchial airways: two-phase flow simulation

Mohammad Rahimi-Gorji, Tahereh B. Gorji *, Mofid Gorji-Bandpy

Department of Mechanical Engineering, Babol Noshirvani University of Technology, P.O. Box 484, Babol, Iran

ARTICLE INFO

Article history:
Received 22 January 2016
Received in revised form
23 April 2016
Accepted 26 April 2016

Keywords:
Micro-particle deposition
Human tracheobronchial airways
CT-scan based images
Computational two-phase flow
Lagrangian particle tracking

ABSTRACT

In the present investigation, detailed two-phase flow modeling of airflow, transport and deposition of micro-particles (1–10 μm) in a realistic tracheobronchial airway geometry based on CT scan images under various breathing conditions (i.e. 10–60 l/min) was considered. Lagrangian particle tracking has been used to investigate the particle deposition patterns in a model comprising mouth up to generation G6 of tracheobronchial airways. The results demonstrated that during all breathing patterns, the maximum velocity change occurred in the narrow throat region (Larynx). Due to implementing a realistic geometry for simulations, many irregularities and bending deflections exist in the airways model. Thereby, at higher inhalation rates, these areas are prone to vortical effects which tend to entrap the inhaled particles. According to the results, deposition fraction has a direct relationship with particle aerodynamic diameter (for d_p=1–10 μm). Enhancing inhalation flow rate and particle size will largely increase the inertial force and consequently, more particle deposition is evident suggesting that inertial impaction is the dominant deposition mechanism in tracheobronchial airways.

1. Introduction

Inhalation and exhalation are the most basic physiological functions required for human body to sustain life. Today, the science of respiration is multidisciplinary; having important contributions from different disciplines of medicine, engineering and basic sciences. There are various processes of human respiratory system such as gas exchange, speech production, particle inhalation and others that can be of interest to researchers from different fields of expertize. The focus of this research is to investigate the air flow behavior and particle deposition in human airways using computational flow modeling. The branching pattern of the airway network is a major factor affecting the deposition of inhaled aerosols. Particle deposition studies in the human airway tree are very significant for characterizing risks of exposure to particulate matter, developing effective drug treatment methods for chronic airway diseases, and calculating dosimetry for occupational hygiene and medicinal treatments [1]. Major challenges need to be overcome to acquire data that is sensitive to lung geometry and function for addressing non-uniformity and asymmetry of particle deposition in the lungs. These challenges are the representation of realistic airway geometry, the imposition of physiological boundary conditions, and the treatment of turbulence [2]. Accurate 3-D models of the human airway network morphology are of great importance in the study of lung deposition patterns of inhaled aerosols. Knowledge of respiratory aerosol deposition rates and locations is necessary to design effective inhaled medications (i.e., aerosol therapy) that target specific lung regions [3,4].

The earliest studies of airflow in the lung airways include experimental works which presented a few velocity profiles and flow patterns for a double bifurcation model [5,6] followed by numerical studies of velocity field, particle trajectories, and deposition efficiency for 2-D and 3-D single and double bifurcations [7], 2-D steady inspiratory airflow through a double bifurcation model representing three generations of the human central airways [8], reconstructing an average geometrical model of the extra-thoracic airways based on data from computed tomography (CT) scans, magnetic resonance imaging (MRI) scans, and direct observation of living subjects [9] and implementation of a simplified, but more complete model of the upper human airways incorporating a bend between mouth and trachea [10] based on data sets provided by cast of human oral airways [11].

Simulation of micro-particle deposition in human airways have shown substantial differences between a realistic geometry and a simplified one; the realistic geometry provided the best predictions

* Corresponding author.
E-mail addresses: m69.rahimi@yahoo.com, m69.rahimi@stu.nit.ac.ir (M. Rahimi-Gorji), gorji.tahereh@stu.nit.ac.ir (T.B. Gorji).

http://dx.doi.org/10.1016/j.compbiomed.2016.04.017
0010-4825/

Nomenclature

x	x coordinate
y	y coordinate
z	z coordinate
u_i	Mean velocity in tensor notation (m/s)
u_g	Fluid (air) velocity (m/s)
u_p	Particle velocity (m/s)
IP	Inertial parameter ($\mathrm{Ip} = \rho d_p^2 Q$)
y^+	Dimensionless cell height ($y^+ = \frac{y}{\nu_f}\sqrt{\frac{\tau_{wall}}{\rho_f}}$)
Re_p	Particle Reynolds number (–)
Re_r	Relative Reynolds number (–)
R_k, Re_t	Model constant of k-ω LRN ($R_k = 6$, $Re_t = \frac{k}{\upsilon_{f\omega}}$)
d_p	Particle aerodynamic diameter (μm)
CT	Computed tomography
MRI	Magnetic resonance imaging
TB	Tracheobronchial
CFD	Computational fluid dynamics
DICOM	Digital Imaging and Communication
STL	Standard Tessellation Language
LRN	Low Reynolds number
FOV	Field of view
C_D	Drag coefficient ($a_1 + \frac{a_2}{Re_r} + \frac{a_3}{Re_r^2}$)
DE	Deposition efficiency (–)
p	Mean static pressure (pa)
a^*, a^*_∞	Model coefficient, k-ω LRN (–)
t	Time (s)
g	Gravity (m/s^2)
F_D	Drag force (N)
K	Turbulent kinetic energy (–)
G_{prop}	Transferred product specification (–)
Y_{prop}	Transferred product specification's loss (–)

Greek symbols

ρ	Fluid density (kg/m^3)
ρ_p	Particle density (kg/m^3)
υ	Kinetic molecular viscosity (μ/ρ)
ω	Specific dissipation rate (s^{-1})
υ_T	Kinetic eddy viscosity $\left(\mu_T/\rho\right)$
υ_f	Fluid viscosity $\left(\mu_f/\rho\right)$
B_i	Model constant of k-ω LRN (–)
μ	Kinetic viscosity (Kg m^{-1} s^{-1})
α_1, α_2, α_3	Model constants of the Morsi and Alexander drag law (–)
σ_ω, σ_k	Model constant of k-ω LRN ($\sigma_\omega = \sigma_k = 0.5$) (–)

of regional deposition in comparison with experimental data and hence are needed for accurate evaluation of localized deposition patterns [12–16]. Studies which focused on patient-specific lung geometries have proved to be more pertinent to clinical issues [17,18].

Recently, Rahimi-Gorji et al. [19] demonstrated airflow behavior and particle deposition in three breathing conditions through a realistic human respiratory system (Trachea-G2). In the present investigation, computational fluid dynamics (CFD) was utilized to investigate the effects of several different breathing conditions on the particle ($dp = 1$–10 μm) deposition in a 3-D realistic human airway model extending from mouth to generation G6 of airways. The geometry reconstruction from CT-scan images was performed using 3D-DOCTOR software. The simulated inhalation rates include sedentary (i.e., 10 L/min), light breathing (i.e., 15 L/min), normal breathing (i.e., 30 L/min), semi-heavy breathing (i.e., 45 L/min) and heavy breathing (i.e., 60 L/min) conditions. For capturing the airflow laminar, transient to turbulent behavior within the airways, the low Reynolds number (*LRN*) k-ω turbulence model was implemented. One-way coupling was used between the continuous phase (i.e., inhaled air) and discrete phase (i.e., injected particle) to track the particles motion.

2. Model reconstruction and grid generation

The airway model includes the oral cavity, pharynx, larynx, trachea, and bifurcating airways representing mouth to G6. The images were obtained from computed tomography (CT) spiral multi-slice scan of a healthy 63 years old, non-smoking male. The slice thicknesses of CT-scan images was set to 0.5 mm and a total of 1023 slices were considered for reconstruction of mouth to G6 using the single-matrix scanner in helical mode, a 500-mm field of view (FOV), 120 kV peak at 50 mA. The CT-scan images – DICOM (Digital Imaging and Communication) files- were imported to 3D-DOCTOR image processing software. The slices were segmented and imported with a Standard Tessellation Language (STL) format to CATIA-V5 software. The STL format file was converted there to CATPART and then to IGES format. There, The IGES file was imported to ANSYS-Workbench 15 (Fig. 1(a)) to create faces, volumes and extended tubes at inlet and outlets. The morphological specifications of the reconstructed patient-specific geometry are listed in Table 1. Since it is noteworthy to avoid reverse flow at the geometry entryways, they should be extended. The segmented computational domain at this stage is shown in Fig. 1(b). The geometry was meshed by structured tetrahedral mesh using the Meshing module (Fig. 1(c)) and the generated mesh was then read into ANSYS FLUENT 15 for numerical simulation. From the zoomed out parts of Fig. 1(c), it can be seen that the angle of the surface tetrahedral grid is smooth enough to generate a high quality volume mesh. Moreover, the triangular distribution is related to the contour of the configuration. More grid nodes are distributed on the region where the profile has acute changes, which can ensure that the reconstructed geometrical model closely matches the realistic situation. Additionally, to fully capture the turbulent boundary layer profile at the near wall regions, 5 prism layers are added to the geometry surface. Based on the implemented turbulence model, the y^+ value for the mesh refinement used was less than 1 ($y^+ < 1$). For studying the grid size sensitivity on the flow solution, different grids consisting of approximately 2,410,000 (Mesh 1), 3,350,000 (Mesh 2), 4,250,000 (Mesh) and 5,100,000 (Mesh 4) cells were implemented and axial velocity profiles at two sections (A, B in Fig. 1(a)) were obtained. According to Fig. 2(b), the increase of grid size from 4,250,000 to 5,100,000 cells does not alter the results and the velocity profiles are overlapped. Hence, a mesh with 4,250,000 grid size was adopted for the simulations.

3. Numerical formulation

3.1. Airflow phase

The governing equations of the flow phase were considered under steady-state, incompressible and Newtonian fluid assumptions. Although the flow structures and subsequently particle