CFD Modeling and Analysis of Pulmonary Airways/Particles Transport and Deposition

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Unsteady numerical simulations of air flow, mixed with micron particles, through a human lung conducting zone during inhalation have been performed. The process included importing images from a high resolution CT-Scan into a CFD software, generation of the CFD model and then CFD simulation over a 4 seconds cycle (2 seconds for inhalation and 2 seconds for exhalation). The inlet diameter was 11 mm and the flow rates were 5, 7.5, and 15 liters/min. Only results for the highest flow rate are presented. The implicit-unsteady Reynolds Average Navier-Stokes equations with the Wilcox K-ω turbulence model were used for the simulation. The micron particles were solid round coal with 1000 Kg/m³ density. Results indicate high correlation between regions of high vorticity and secondary flow and particle deposits. This was mostly evident in the main bronchus. While most particles should exit the lung during the exhalation process, however, areas of recirculating flow and near the walls continue to have some particle deposits.

I. Introduction

The present investigation is part of a joint project between the Center for Energy and Environmental Research and Services (CEERS) at California State University, Long Beach (CSULB) and the Pulmonary Division of the Veterans Administration (VA) hospital in Long Beach, California, for development of a patient specific non-intrusive diagnostic system of human respiratory system using computational fluid dynamics (CFD). The method could also provide detailed understanding of the impact and deposition of the inhaled particulate matter (PM) on human lung function, development of enhanced drug delivery systems and improved preventive measures for controlling the quality of the inhaled air. Physicians currently have to use two to three different modalities to evaluate a patient lung. The difficulty lies in the anatomic versus functional evaluations. The main resource used to evaluate a patient's functional capacity is a Pulmonary Function Test (PFT). The method is labor intensive for both the patient and the medical system and some patients are so debilitated that the study could not be performed. The PFT tests results are used to quantify the functional extent of the patient disease and its prognosis. Physicians also use ventilation/perfusion lung scan (V/Q scan), on a limited basis, to determine lung function. These studies are even more labor intensive than the PFT studies. Currently the primary modality used for lung anatomical evaluations are Computed Tomography (CT scans). They are reliable, fast and extremely effective for anatomical lung evaluations but provide no information about a patient’s functional capacity. Physicians are currently stuck performing multiple different studies to get a true evaluation of the extent of disease of a patient.

A CFD-based diagnostic system provides physicians with the possibility of obtaining both functional and anatomical data, having only utilized one diagnostic resource. With an easily obtained CT scan and the addition of CFD modeling it's possible to evaluate a patient's pulmonary status leading to prognostic and therapeutic interventions. This would decrease both patient and healthcare resource utilization without decreasing effective healthcare delivery.

There are strong evidences that inhaled pollutants can have adverse impacts on lung and heart. It is also possible that the inhaled particulates travel into the brain along nerves from nasal passages and/or be transported via the blood stream from the lungs. Clinical studies on dogs and mice have shown significant increases in the levels of inflammatory markers and abnormal protein deposits in the brain of animals that are exposed to high

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levels of particulate matter (PM) [1]. These markers and abnormalities are also seen in patients with antecedent clinical features prior to the onset of the Alzheimer’s disease. Although further clinical studies and research are needed to assess the exact impact of air pollution on the brain, these studies show that the brain is not immune to ambient air pollution.

Understanding the role of micron and nano particles on respiratory systems and ways to reverse their impacts are of major interests to scientists, healthcare provider and engineers. For the research scientists and healthcare providers, the simulation can provide a diagnostic tool to assess how the micron and nano particles transport, diffuse and deposit throughout the human lung, identification of the dysfunction areas, and development of drug aerosol delivery system for treatment of targeted areas. For engineers and policy makers, it provides information about the particles characteristics and their level of concentrations that results in lung disability and preventive measures and policies that should be enacted to prevent such depositions and the subsequent adverse health impacts. Asbestosis and silicosis are among the occupational diseases that inflame the lung tissues, leading to fibrosis.

Human lungs are one of the body’s largest organs. Their function is gas exchange, delivering oxygen and removing wasted carbon dioxide. Air enters the body through nostrils and mouth into trachea, which is then divides into left and right primary bronchus. The bronchus branch out into secondary bronchi and then each subdivides into tertiary bronchi and so on, reducing diameter throughout the structure until the respiratory bronchioles which distribute air to the alveoli.

Flow through the pulmonary airways could be laminar or turbulent. Turbulent flows may occur during elevated inhalation flow rates, during exercises or due to partial pulmonary dysfunction. In addition branching in the conducting zone may cause pressure drops and result in local turbulence spots. In the respiratory zone, flow is dominated by laminar and diffusion flows.

During the exhalation process, the merging flows from the branches might result in pressure recovery and unsteadiness, leading to oscillation. In both inhalation and exhalation processes, there are areas of secondary flows which significantly affect the motion of the particles and the impaction processes. Other factors that contribute to the particle motion and impaction are diffusion and the gravitational effects.

There have been extensive studies in modeling the lung function using CFD. Developed theoretical models have been either symmetric (2-5) or asymmetric (6). However, these general models do not take into account the irregularities that every lung could have. Some researchers (7-11) have focused on patient-specific lung geometries and their results are more pertinent to the clinical results. However, significant progress is needed, before a realistic diagnostic system could be developed. Reference 12 provide extensive and up to date reviews on modeling of the pulmonary airways.

The particle transport is governed by the Newton’s second law of motion where the acting forces are the drag and gravity forces and the near wall stresses. The convection-diffusion of particles is governed by the Navier-Stokes equation for scalar particle and the Fick’s law of diffusion.

In previous studies (13, 14), the boundary condition at the inner surface has been defined as:

\[ \nabla \cdot (D \nabla c) = -D S (\nabla c) \] 

Here, D is the coefficient of diffusion, S is the surface area, \( \nabla c \) is the gas concentration gradient, and \( \nabla \) is the average gas exchange rate over the respiratory cycle. The surface area is assigned according to the lung surface condition and thus the exchange rate is estimated.

II. Model and Analyses

Accurate CFD analysis of the lungs is based on modeling of different zones of the respiratory system. To achieve this goal, MRI and CT scans have been converted into three-dimensional models with the 3D-Doctor visualization software. Scans were imported in DICOM file format and through color contras and complex surface rendering, raw images from 2D cross-sections were used to define the required boundaries and generate the 3D model (Figure1a.) which is then transferred (in STL format) to the STAR CCM+ CFD software for simulation and analyses.

Figure 1b illustrates the difference between 2 patients’ trachea and bronchial tree up to 5th Generation of lung. In this paper a set of CT scans from patient 1 was intentionally chosen to understand the effect of geometry on the deposition of PM particles.
The numerical investigations were performed using the implicit unsteady Reynolds-Averaged Navier-Stokes equation (U-RANS) using the commercially available software (STAR CCM+) from CD-Adapco with Wilcox K-ω turbulence model (15). Segregated flow condition with various input functions for specific conditions were used. The initial and boundary conditions were as follow:

Initial conditions:
• Turbulence: intensity: 0.01 (1%)
• Turbulence: Length scale: 1.5 mm

Boundary conditions:
a) Velocity Inlet: 0.868-1.3-2.603 m/s
b) 18 pressure outlets: pressure difference = -6 to -15 pa (Pressure at the outlets must be known priori [16]. CFD simulations of patient-1 lung showed pressure drop of 6-15 pa at 5 to 15 L/min at 5 generation branches of the lung).
c) Wall: stick physical boundary condition has been chosen to mimic the effect of mucus layer in trachea and primary bronchi

The introduced micron particles for the Lagrangian phase of the study had the following properties:
• Particle density: 1000.0 kg/m³, spherical particles
• Mass flow rate: 1.25*10⁻¹³ kg/s to 3.75*10⁻¹¹ kg/s
• Particle diameter (dₚ): 1, 5, and 10 µm
• Velocity: same as inlet velocity

Investigations have been performed for three inlet volumes of 5, 7.5 and 15 liters per minute. However, due to limited space, results are presented only for the 15 liters/min inlet volume with 10 µm particles.

III. Results and Discussions

Inhalation Process

Figures 2 and 3 show cross sectional views of the mean velocity, velocity vectors, and turbulent kinetic energy (TKE) of the lung, at different locations. Figure 4 shows the axial sectional view of the mean velocity and the TKE within the trachea. The inlet section mean velocity contours show increased velocity near the wall which decreases downstream but with increased velocity gradient. Secondary flows are observed within the trachea and with approaching of the first branch. There is an uneven distribution of the mean velocity between the branches. Turbulent kinetic energy is increased as the air passes through the curved sections of the trachea which include the regions of the secondary flows.
The axial sectional views of the trachea show relatively uniform mean velocity and TKE at the inlet. The mean velocity accelerated through the curved section with higher velocity gradient near the lower wall and then decreased mean velocity and TKE downstream. There are regions of low velocity and secondary flow after the curvature. The increased velocity gradient and TKE created added stress on the lung wall region and the secondary flow regions have potentials for particle deposits.

Figure 2. Mean Velocity Contours and Velocity

Vectors at Different Sections of the Lung.

Figure 3. Contours of Turbulent Kinetic Energy

Figure 4. Velocity Magnitude and Turbulent Kinetic Energy within Trachea.

Figure 5 shows regions of the particle deposition, when particles are introduced at the trachea inlet. Figure 6 shows the vorticity regions. Particle depositions are seen in high curvature areas and at the inlet to the branches. These locations are also regions of high vorticity. Figure 7 shows the corresponding results for wall shear stress with particles shown, which indicate concentration of the particles within high stress regions.
Figure 5. Particle Depositions during the Inhalation Process.

Figure 6. Variation of the Vorticity within the Lung.
Figure 7. Variation of the Wall Shear Stress.

The incident mass flux of the particles along the surfaces can be assessed with the deposition factor \((DF)\) which can be calculated as:

\[
DF = \frac{\text{Total number of particles deposited}}{\text{Total number of particles introduces}} = \frac{\int \text{Incident mass flux of lagrangian phase}}{\text{Mass flow rate of particles at inlet}}
\]

Figure 8 shows variations of the percent particle deposits with stoke number \((St)\), which is related to the behavior of the particle suspended in the flow. It is defined as:

\[
St = \frac{\rho_p d_p^2 U}{18 \mu D_{in}} \quad (2)
\]

The deposition factor is represented in terms of dimensionless stoke number \((St)\), which is related to the behavior of the particle suspended in the flow. It is defined as:

\[
St = \frac{\rho_p d_p^2 U}{18 \mu D_{in}} \quad (2)
\]

Equation 1 provides a mean of estimating the gas exchange rate, according to the local gas concentration gradient. It is expected that those areas with particle deposits have reduced gas exchange rate due to reduced gradient. In addition, the local velocity gradients can be used as a diagnostic tool in assessing the conditions and capacity of specific lungs as related to the various pulmonary diseases.

**Exhalation Process**

Figures 9-11 show sectional variations of the mean velocity, velocity vectors, vorticity, TKE, and wall shear stress. The variations are provided for two axial sectional views as indicated on the graphs. The mean velocity and the velocity vector plots indicate increased velocity near the wall through the curved section, opposite to the location during the inhalation process. There is a region of low velocity and weak secondary flow beyond the curved section, before the air exits the lung. There is no significant vorticity and the TKE is high only in regions where flow from various branches merge. Similar results are seen for the wall shear stress. These results indicate that while some of the micron particles deposit into the lung surface during the inhalation process, however, most will exit and only those shown during the inhalation at the lung surface are expected to remain. Due to difficulty in resolving movements and release of particles during the exhalation process, the corresponding results for the PM distribution have not been provided.
Figure 8. Variation of the Deposition Factor with Stokes Number.

Figure 9. Sectional Views of Mean velocity (a, b) and Velocity Vectors (c).

Figure 9. Sectional Views of Mean velocity (a, b) and Velocity Vectors (c).
Figure 10. Sectional Views of Vorticity (a) and TKE (b&c)

Figure 11. Sectional Views of Wall Shear Stress.
Unsteady simulation of a patient lung during the inhalation/exhalation cycle has been performed. The simulation was for 4 sec. at a volume flow rate of 5, 7.5, and 15 liters/min. During the inhalation process, micron particles with a density of 1000 Kg/m$^3$ and a mass flow rate of 1.25*10^{-11} to 3.75*10^{-11} kg/s were introduced into the air inlet and the effects of the geometry and flow conditions on particle depositions have been analyzed. The simulations identified regions of flow acceleration, recirculation and reduced velocity and results show that areas with high vorticity and at the inlet to the branches are candidates for high rate of particles depositions. Due to simulation difficulties, the corresponding results for the exhalation process were not available, however, simulations of the exhalation indicate very limited areas of high vorticity and secondary flows which implies except for those depositions where exhalation could not impose high rate of flow and particles are attached to the surface, the remaining particle should exit the lung. This condition could be different for different patients.

References