Air Quality Index Effect on Particles Deposition in Human Respiratory Tract under Natural Breath

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Abstract. The huge demands of material goods decayed the breathing air quality. Now, it is reflecting on the clinical respiratory test of humans. Therefore, it is a serious issue that needs to be taken care of. The article throws-up light on important factor such as a deposition of inspired toxic particles under natural breath. The inspired particles are having an aerodynamic diameter 2.5 µm and 10 µm. A three-dimensional CT-scan based Human Respiratory Tract is successfully re-constructed nasal cavity to 7th generation bronchi. The flow is developed during inhalation laminar to turbulent from external nostrils to the tracheobronchial airway due to anatomical effect. It is affected the particles deposition on the various regions due to inertial impaction or curved shape surface of the airway model. The appropriate turbulence model quantifies the internal flow features so that an accurate trajectory of particles transport pattern can be presented. The discrete phase model (DPM) is used for particles tracing on Language frame, which gives the combined effect of anatomical structure and airflow impact on the deposition of particles. It could be useful for the diagnosis of Human airways illness.

Keywords: Air quality index (AQI), Computer tomography (CT), Human Respiratory Tract (HRT), Computational fluid dynamics (CFD), Discrete phase model (DPM).

1. Introduction

The inhaled micro-size particles deposited into the Human airways. In Asian countries, many states peoples are breathing air below the safety standards. According to the national air quality index in India. The breathing air quality index should below for PM$_{2.5}$ (41 µg/m$^3$) and PM$_{10}$ (154 µg/m$^3$). In the particle deposition analysis, nasal cavity played a vital role. Nasal cavity is the prime defence mechanism which filters the inspired air before distributed into the Human airways. However, in that mechanism, the anatomical structure of airways has put great influence on particle deposition. The minor changes in the airway structure are putting a significant effect on particle deposition and characteristic flow (laminar, transitional and turbulent) on different segments [1]. The sudden expansion and contraction in airway passage are increasing the deposition efficiency due to inertial impaction and also increases the computational efforts [2]. With the Weibel model it is very difficult to predict the realistic particle deposition efficiency and airflow characteristics [3]. However with the different breathing conditions, breath hold of 2 s, cannot accomplish particle deposition efficiency in the airway. But it definitely increases deposition efficiency in the bifurcation junctions [4, 5]. The particles deposition efficiency is connected with the inertial force of particles. It is a key factor for the small sizes particles deposition [6]. The particles deposition efficiency in diseased airway relatively with high Reynolds number flow comparing with the asthmatic and healthy airway. Also it is decreasing the lungs function mechanism [7]. The micro-sized particle deposition efficiency is higher in comparison of nano-size particles in the airway [8]. The maximum deposition efficiency was occurs at a high airflow rate during inhalation [9]. In past studies, the particles deposition in-vitro and in-vivo model including with the different size of particles listed in the literature. Although, steady-state numerical findings are reported. The particle deposition with the natural breath in-vivo model of nasal cavity was found very less. Also, in this regards many health risk studies were performed without considering the AQI and natural breathing. The article concern the importance of particle deposition in the HRT model at moderate and very unhealthy AQI. There is no literature available on such a topic. The numerical results are presented the regional particle transport and deposition pattern during peak inspiratory airflow.

2. Human Respiratory Tract Model and Grid Generation

The total 1024 number of CT-scan slices arranged together. The field view of slices 31.60 cm and a pixel size of 0.623 mm. The three-dimensional mask of selected images are created by changing the Hounsfield Unit (HU) (-1024, -200) of tissues. The airways model is ready for computer graphical user interface. In figure 1 the three-dimensional HRT model is shown with descriptive validation.
To discretize the flow domain the unstructured grid is constructing using “ICEM” software. The grid indecency test is performed for the grid elements size of 4.5 mm, 4 mm, 3.5 mm and 3 mm at the airflow rate of 30 L/min. The numerical grid is independent in 4 mm element size. The final grid is having 68, 90,000 elements.

3. Numerical Methodology

The Natural breathing airflow (10 L/min) is simulating shown in figure 2. The following assumptions are considered, (1) Unsteady state incompressible flow, (2) Flow domain wall considered as rigid hydraulically. The conservation of mass (continuity equation) and momentum equation can be written as:

\[ \frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0 \]  \hspace{1cm} (1)

Momentum equation:

\[ \frac{\partial u_i}{\partial t} + \frac{\partial (u_i u_j)}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \frac{\mu}{\rho} \frac{\partial^2 u_i}{\partial x_j \partial x_j} \]  \hspace{1cm} (2)

Where \( \mu \) is the dynamic coefficient. The \( u_i, u_j \) (i, j = 1, 2, 3) are velocity components in the cartesian coordinate in x,y,z directions. The \( p, \rho, \nu \) stand for the pressure, air mass density (\( \rho = 1.25 \text{ kg/m}^3 \)) and kinematic viscous coefficient of air.

3.1 Assessments of Turbulence Model

The (Realizable) \( k-\varepsilon \) model investigates the detailed internal flow information of airways. The similar turbulence model was used [10] in past research. The turbulence model transport equations for \( k \) and \( \varepsilon \) in the realizable are:

\[ \frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_j} (\rho u_j k) = \frac{\partial}{\partial x_j} \left[ \left( \frac{\mu}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + \frac{\partial}{\partial x_j} \left( \rho C_i S_j \right) + G_k + F_k - Y_k + S_k \]  \hspace{1cm} (3)

\[ \frac{\partial}{\partial t} (\rho \varepsilon) + \frac{\partial}{\partial x_j} (\rho u_j \varepsilon) = \frac{\partial}{\partial x_j} \left[ \left( \frac{\mu}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + \rho C_s \varepsilon - \rho C_\varepsilon \varepsilon + \rho C_\varepsilon \varepsilon - C_{\mu} \frac{\varepsilon^2}{k} + C_{\mu} \frac{\varepsilon}{k} C_{\mu} S + S_{\varepsilon} \]  \hspace{1cm} (4)

Where constant:

\[ C_i = \max \left( 0.43, \frac{n}{n+5} \right) \]  \hspace{1cm} (5), \[ C_\varepsilon = 1.9 \]  \hspace{1cm} and \[ C_{\mu} = 0.09 \] , where, \( S \) is the modulus of the mean rate of strain tensor, defined as \( S = \sqrt{2S_{ij}S_{ij}} \) \hspace{1cm} (6), \( \mu \) is the dynamic viscosity of the fluid. Eddy viscosity of the fluid \( \mu_e \) is given as \( \mu_e = \rho C_{\mu} \frac{k^2}{\varepsilon} \) \hspace{1cm} (7), the \( k-\varepsilon \) turbulence model appears to be capable of reproducing the limiting laminar and fully turbulent flow.

3.2 Discrete Phase Model

To solve the trajectory of particles are considering the effect of drag force and gravity at integrating force balance equation, therefore numerical equation is written on a Lagrangian frame.
\[
\frac{du}{dt} = F_D(u - u_p) + \frac{g(\rho_p - \rho)}{\rho_p} \quad \ldots \ldots (8)
\]

Here, \( U \) is the fluid velocity. \( U_p \) is the particle velocity. \( \mu \) is the molecular viscosity of the fluid. \( \rho_p \) is the density of the particle. \( d_p \) is the particle diameter. Where \( F_D(U - U_p) \) is the drag force per unit injected particle mass in the airway model, written as

\[
F_D = \frac{18\mu C_D \text{Re}}{\rho_p d_p^2} \quad \ldots \ldots (9)
\]

\( \text{Re} \) is the relative Reynolds number, written as

\[
\text{Re} = \frac{\rho d_p |u_p - u|}{\mu} \quad \ldots \ldots (10)
\]

The density of particles is considered as equivalent to water (1000 kg/m\(^3\)). The mass of PM\(_{2.5}\) and PM\(_{10}\) are injecting according to moderate and very unhealthy AQI.

### 3.3 Numerical Schemes

The individual velocity inlet UDF (10 L/min) is defined at both nostrils with hydraulic diameter 0.0141 m and 0.0126 m left and right nostril respectively. The trapped boundary conditions are imposing on the flow wall. At the inlet and all outlets defined as reflecting boundary conditions. Zero-Gauge pressure has established at the outlets. The internal fluid dynamics is simulated by the finite-volume based solver. The pressure-velocity coupling SIMPLE-C was adopted. The QUICK transport equations were discretized up to second-order accurate in space. The adaptive time method is used to capture the local features of the airway.

**Figure 2.** Natural breathing profile for normal volumetric flow (10 L/min).

### 4. Results and Discussions

#### 4.1 Particle Transport and Used Turbulence Model Comparison

The transport and deposition efficiency of particles in the nasal cavity is compared with the experimental results of Kelly et al. [11] shown in figure 3 (A). The CT-scan based nasal cavity is used for the validation. It is necessary to know the quantified value of particle mass deposited inside the airway. The regional deposition efficiency is a good parameter. The deposition efficiency is defined as the ratio of particle mass deposited in the trap region/mass of particles injected. In HURT model, the sudden anatomical changes occurred. If the flow magnitude is increasing due cross-sectional area the particle deposition efficiency increases due to inertial impaction (IP). The overall CFD results are showing reasonable agreement with experimental data. Also during inhalation, the higher resistances occurred at the nasal valve because of narrow cross-section. Which means pressure drop occurs at the nasal valve in [12]. The flow validation is carried out with the computational results of Wang et al. [10]. The average pressure drop is calculated at the nasal valve with various inspiratory airflow rate. The flow characteristics show a good agreement with the simulated results are shown in figure 3 (B).

#### 4.2 Inspired Particles Transport and Deposition Pattern

In figure 4 show the airflow streamlines and transport pattern of the inspired particles at moderate and very unhealthy AQI for PM\(_{2.5}\) and PM\(_{10}\) during peak inspiratory flow at \( t = 2.1 \) s. The particles flow inertia, geometrical shape and gravitational force are affected the transport pattern of particles within the airways.
During normal breathing, airflow is laminar [13] in the nasal cavity. As the airflow magnitude increases in distinct segments of airways.

![Figure 3](image1)

**Figure 3.** (A) The deposition efficiency in the nasal cavity due to the inertial mechanism, (B) The avg. pressure drop across the nasal valve during inhalation.

The particles deposition efficiency is varying due to asymmetric velocity inlet. It is observed that initially, the left and right nostril particles transport pattern are not similar. Although inspired air is the carrier for the injected mass of inspired particles. As the airflow streams are moving the particles also moving and deposited on the flow wall as come in to contact due to mucous. The airflow streamlines interact with the transport pattern in the middle turbinate and olfactory region. As increasing the AQI (201-300) the transport pattern of particles is changed in the nostrils and olfactory region as well. The airflow is progressed towards the nasopharynx region flow streams are merging in that region. Which is coming from both the nostrils cavities. Due to the sudden proximal bend of 90° particles start accelerating because of high flow magnitude. The anatomical structure of pharynx has influenced the transport and deposition patterns. Due to high flow velocity magnitude, the particle is concentrating middle of the glottis because of the nozzle effect it is moving towards the anterior side of the pharynx. The deposition of particles must be increased in pharynx larynx. The trachea has a straight pipe. But in the real model, it has the cartilage rings which is affecting the airflow streamlines locally.

![Figure 4](image2)

**Figure 4.** The inspired particles transport pattern and velocity streamlines during moderate and very unhealthy AQI for PM$_{2.5}$ and PM$_{10}$ at [t = 2.1 s] respectively: (a) Front view. (b) Isometric view.

Therefore at the entrance of trachea, the particles influenced by glottis nozzle effect. In the other side the development of inspiratory flow in trachea prominently particles concentration at the posterior side. Also, the particles transport pattern shifted towards the right side instead of left side bronchus and low flow velocity zone.
is formed in the right side before the first bifurcation seen in figure 4. The inspired particles are non-uniformly strike to main bronchus carina and partitioned left and right main lungs asymmetrically. However, the inspired flow inertia is the primary mechanism to penetrated particles in subsequent branches of lungs. Therefore more mass of inspired particles transported and deposited in the left lungs that’s why total deposition efficiency is higher in left lungs bifurcation. The PM$_{10}$ particles trends are different as compared with PM$_{2.5}$. It shows a higher deposition in the upper airways. The particles deposition efficiency is compared for 2.5 $\mu$m and 10 $\mu$m particles. The left lungs have higher deposition efficiency 1.2% as compared to right lungs during AQI (51-100) similarly as increase the AQI (201-300) it is increasing up to 1.38% for PM$_{2.5}$. Also for PM$_{10}$, it will become 2.24% higher in left lungs during AQI (51-100) and 2.48% during AQI (51-100) and AQI (201-300) for PM$_{10}$. At a particular instant significant differences occurred in transport and deposition pattern of particles in airway after changing AQI moderate to very unhealthy.

Conclusions
The current study shows the following conclusions.
1. The anatomical structure of HURT model distinct the transport pattern of injected mass in left and right side nostrils in moderate and very unhealthy AQI.
2. The development of airflow in the trachea, the inspired mass of particles shifted towards the right side because of low flow velocity zone in trachea. The particles are deposited in left lungs.
3. The higher deposition efficiency is found in daughter branches due direct impact of mass on cranial. The prominent difference occurred in deposition of particles after changing the AQI moderate to very unhealthy.

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