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Original scientific paper

Transient Numerical Simulation of Airflow Characteristics in the Mouth-Throat 3D Model

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Abstract: Air pollution is a public health problem that has a serious effect on human health, as it leads to increased morbidity and mortality. Each year, more than 3 million people die from air pollution, while many more have higher risks of stroke, heart attack, and lung diseases as a result of the pollution. The available epidemiological studies indicate that exposure to particulate matter in the air can have a toxic effect on the cardiovascular system, and increase the death risk from cardiovascular diseases such as ischemic heart disease and heart failure. In this study, we have reconstructed the upper respiratory tract model from the CT images in order to analyze airflow patterns during the inhalation part of the breathing cycle and to track NO_2 particles inhaled through the mouth or nose. The numerical analysis has been performed using the computational fluid dynamics (CFD) method and the discrete particle method (DPM). The continuous phase flow was solved using the *k-ω* Shear Stress Transport model with low Reynolds number corrections.

Keywords: airflow characteristics; computational fluid dynamics; discrete phase model; mouth-throat model; NO_2 particles

1 INTRODUCTION

Air consists of nitrogen gases (78.084%), oxygen (20.946%), argon (0.934%), as well as small amounts of other gases, primarily carbon dioxide, helium, and neon [1]. The air we breathe, in addition to the previously mentioned elements, contains particles and vapors that arise from natural and anthropogenic sources. We inhale millions of particles during each inhalation, and so the surface of our respiratory tract is constantly exposed to various air pollutants [2]. Air pollution has been associated with an acute increase in mortality and morbidity, primarily in the elderly, children, and persons with pre-existing respiratory and cardiovascular diseases [3, 4]. Air pollution has been also associated with more than 3 million deaths per year [3].

Air quality and the type of particles contained in it are very important for our health. Particles of certain chemical compositions can have a negative effect on the health of humans. The most common pollutants include airborne particulate matter (PM) as well as carbon monoxide (CO), carbon dioxide (CO_2), nitric oxide (NO), nitrogen dioxide (NO_2), and sulfur dioxide (SO_2) [3, 5]. NO_2 primarily gets in the air from automobile engines and can lead to airway irritation, coughing, and difficulty with breathing [6]. If inhaled at a high concentration it can lead to pulmonary edema [4] and can contribute to the development of asthma. It was reported that long-term exposure to NO_2 can affect the sense of smell and can lead to chronic lung disease [7]. The negative effects of the particles we inhale can affect any organ or tissue in the body, but most commonly lead to problems with the respiratory system. Air pollution has been found to elevate existing heart conditions, while cardiovascular diseases have been found as the primary cause of deaths due to air pollution [3]. Exposure to $PM_{2.5}$ particles increases the risk of ischemic heart disease, myocardial infarction, and heart failure [8-10]. The air pollution that is the result of traffic has been connected to the left and right ventricular hypertrophy. One of the most common air pollutants related to traffic is NO_2 [11].

The main function of the respiratory system is gas exchange. It is functionally divided into conducting and respiratory zone, while anatomically is divided into the upper and lower respiratory tract. The average adult at rest inhales and exhales about 500 ml of air every 4 seconds. People who are more physically active inhale a much larger amount of air. Inhaled air comes into contact with about 10 m^2 of alveolar walls that are constantly exposed to the air and the pollutants contained in it [12]. The inhaled pollutants can escape or be absorbed by the respiratory tract during the breathing cycle. The particles that have been absorbed can lead to a number of diseases as they initiate inflammatory processes in our bodies [13].

Technological advancement has allowed for improved knowledge related to airflow characteristics and particle transport in the respiratory models. The first studies in this area of research focused on the simplified airway models [14-16] while nowadays researchers have been using patient-specified geometric models developed from CT scans [17-21]. These complex models provide additional information related to airflow characteristics and particle transport and deposition. During breathing, air enters and exits the respiratory tract through the nose and mouth. The distribution of air inhaled through the nose and mouth changes depending on the activity [22]. Although flows are hard to measure in vivo, they are considered to be laminar [23, 24] or more commonly turbulent [16, 25-28]. When it comes to the turbulent flow, a variety of models have been used: *k-ω* [21, 29]; Large Eddy Simulation (LES) [30-32]; *k-ε* [33]; Reynolds-averaged Navier–Stokes (RANS) [30]. Besides analyzing airflow in the respiratory system of healthy individuals, the same approach has been used to determine airflow characteristics in specific diseases such as asthma, chronic obstructive pulmonary disease, and sleep apnea [34-36]. In order to assess drug or air pollutant deposition, it is necessary to perform particle tracking. The understanding of local deposition allows us to better address pulmonary health risks. A number of studies have been performed related to the prediction of particle deposition in the upper respiratory tract [15, 28, 37-39].

Considering the effect of air pollution on health, we have analyzed airflow patterns during the inhalation part of the breathing cycle and tracked NO_2 particles inhaled through the mouth or nose. A realistic 3-D model of the human upper respiratory tract was developed for CT scans. This model was used to perform numerical analysis of the airflow field using the *k-ω* turbulent model and to analyze

NO_2 micro-particle deposition using the Lagrangian method to trace the particles. The aims of this paper were: i) to analyze the airflow in the upper respiratory tract and ii) to track NO_2 particles in the upper respiratory tract under the physiological boundary conditions that correspond to the inhalation part of the breathing cycle.

2 MATERIALS AND METHODS

2.1 Realistic Upper Respiratory Tract Geometry

In order to model the airflow and the movement of the particles in the upper respiratory tract, the volumetric model had to be created. The goal of geometry reconstruction is to create realistic anatomical 3D geometry based on patient images. To achieve this, available software tools were used that allow manual and automatic segmentation of desired domains from computerized geometry images as well as additional optimization of the generated model in order to create a better mesh necessary to obtain more accurate results when applying numerical methods. The upper respiratory tract model was generated using 209 2D axial sections CT scans. The resolution of the used scans was 512 × 512 pixels with slice increment and thickness of 2 mm. The generated model is presented in Fig. 1.

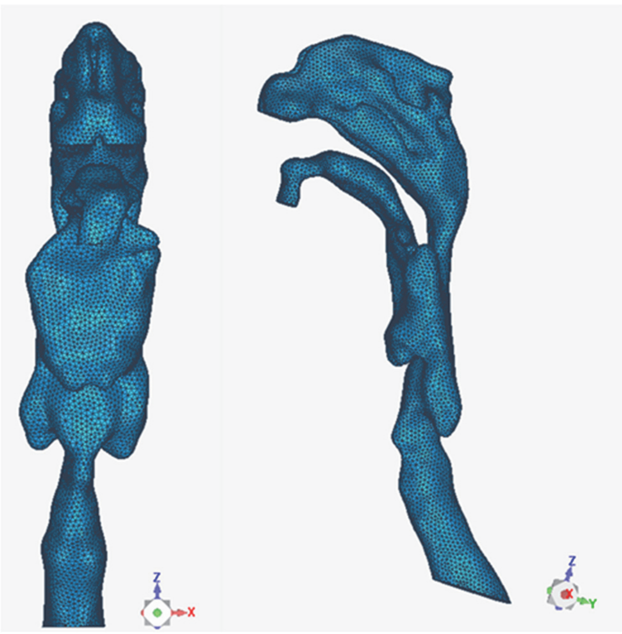

Figure 1 Developed upper respiratory tract 3D model

2.2 Boundary Conditions

Time-dependent airflow simulations were performed using commercial software (Fluent 19 R2, ANSYS, Inc.). Two simulations were carried out (Fig. 2): a) the mouth opening was considered to be a velocity inlet and b) the nose opening was considered to be a velocity inlet.

Respiratory flow in the upper respiratory system was considered to be turbulent and the air was assumed to be incompressible. For this type of respiratory flow, we have used a two-transport equation model that solves equations for the kinetic energy k and specific turbulent dissipation rate or turbulent frequency ω. The k-ω SST (Shear Stress Transport) model with low Reynolds number corrections was adopted for the turbulent flow of air in the upper respiratory tract. This approach has shown an accurate correlation with experimental data [40]. We considered the turbulent intensity value of 5% and a turbulent viscosity ratio of 10. The boundaries of the upper respiratory system were treated as a wall, with a no-slip condition. The SIMPLE scheme was used for the pressure-velocity coupling.

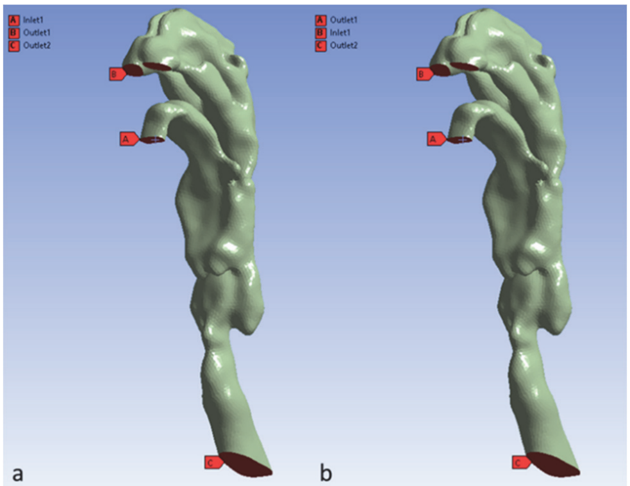

Figure 2 Overview of inlets and outlets used for two simulations

Boundary conditions for each simulation included one inlet and two pressure outlets. Flow in the inlet was normal to the inlet surface area and the velocity was calculated to correspond to the flow rate of 30 l/min. For both velocity inlets, a function for a sinusoidal velocity was defined in a duration of 2.5 s cycle. Although during breathing there is the movement of the wall, it was not considered in this study. Additionally, gravitational acceleration was included.

For particle simulation, Discrete Phase Model (DPM) was considered. Particles were injected using the face normal direction at the mouth (Simulation A) or nose (simulation B) inlet. The Rosin-rammler diameter distribution of inert particles was considered. According to Milenkovic [41], the interparticle collision can be omitted if the particle volume fraction is less than about 10-3. It was assumed that particles in contact with the wall will stay "trapped", while the particles that reach any outlet surface will "escape". The particle trajectories were obtained using the spherical nonlinear drag law implemented in ANSYS Fluent.

3 RESULTS AND DISCUSSION

3.1 Airflow Characteristics

The airflows characteristics were calculated for the inhalation phase of the breathing cycle, for mouth and nose inlets. The presented results, for both mouth and nose inlets, correspond to the peak inspiratory flow. The velocity profile when the mouth was considered for velocity inlet can be seen in Fig. 3. The obtained values were in the range from 0 to 9.5 m/s. Considering the mouth inlet, 0 m/s velocity was expected in the nasal cavity. Based on the literature, higher values were expected in the pharynx and larynx segments of the model. This could be the result of the geometry of the mouth inlet. The velocity profile for the nose inlet can be seen in Fig. 4, where the velocity values were in the range from 0 to 10 m/s.

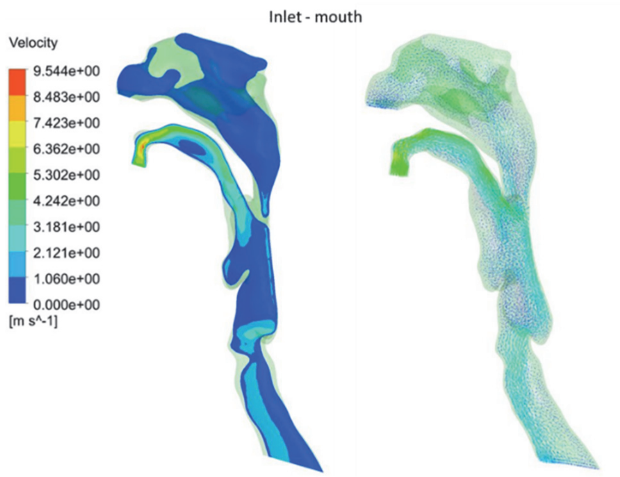

Figure 3 Airflow velocity distributions in the upper respiratory tract for the mouth inlet

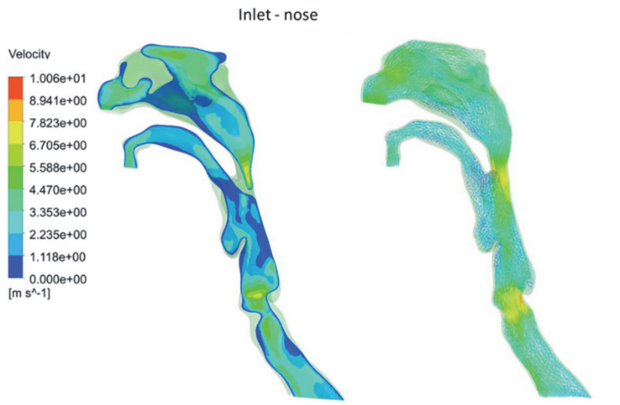

Figure 4 Airflow velocity distributions in the upper respiratory tract for the nose inlet

Although the highest values were in a similar range, it can be noticed that the location was significantly different. In the case of the mouth inlet, the highest velocity was obtained near the mouth inlet (Fig. 3), while in the case of the nose inlet (Fig. 4) the highest values were obtained in the pharynx and larynx segments of the upper respiratory tract, which is in accordance with the literature [42, 43].

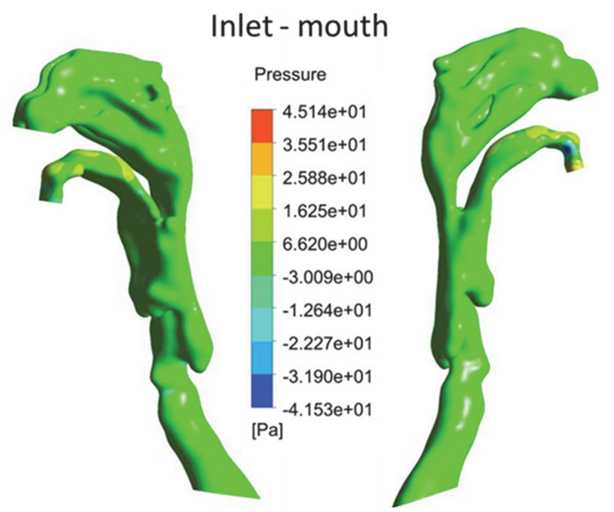

Figure 5 Pressure distribution for the mouth inlet

In order to transport air from the mouth or nose to the lower respiratory tract, a pressure gradient is necessary [44]. This pressure is also important for the deposition of aerosol in the respiratory tract [45]. The pressure distribution for the upper respiratory tract when the mouth was considered as the inlet is shown in Fig. 5.

The pressure distribution when the nose was considered as the inlet is shown in Fig. 6.

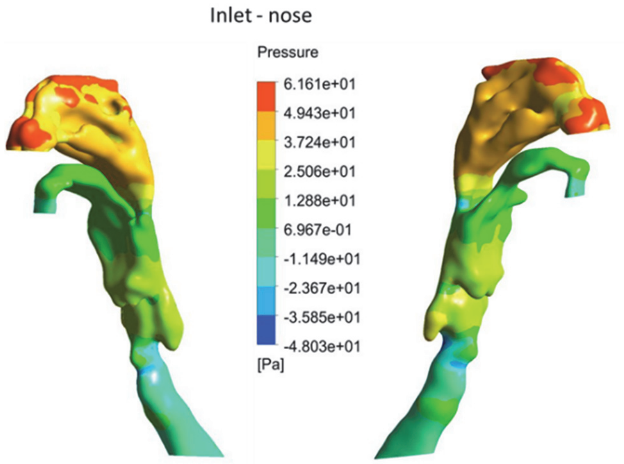

Figure 6 Pressure distribution for the nose inlet

Our numerical simulation indicated pressure variation of 86 Pa for the mouth inlet (from −41 to 45 Pa) and 109 Pa (from −48 to 61 Pa) for the nose inlet. These results were obtained during peak inspiratory flow of the inhalation cycle, corresponding to the normal breathing conditions of an adult. The obtained pressure difference for the nose inlet is comparable to the results in the paper [46]. The pressure change for the mouth inlet is located in the oral area, while in other segments it is very small. In the case of the nose inlet, the highest pressure change was noticed in the nasal cavity.

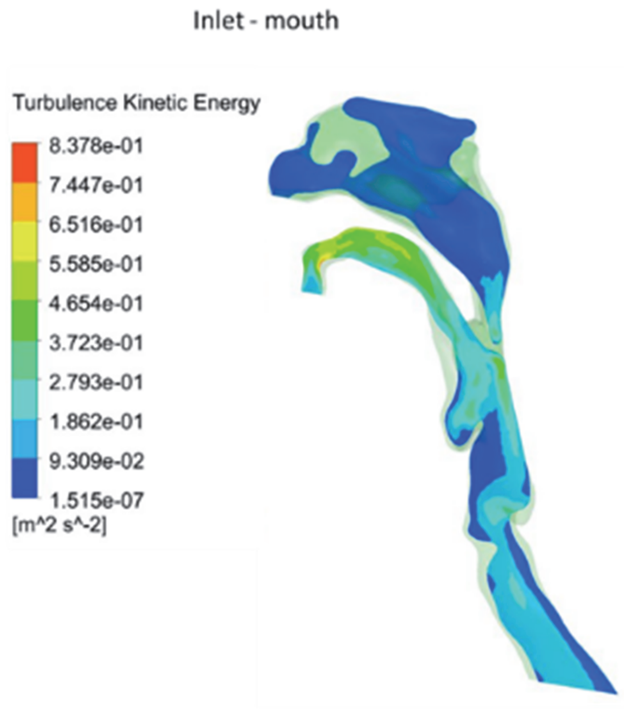

Figure 7 Turbulence kinetic energy for the mouth inlet

Figs. 7 and 8 show the contours of the turbulent kinetic energy at a crosssection for the upper respiratory tract when the mouth and the nose were considered as the inlet. For the mouth inlet, the turbulent kinetic energy decreased as the airflow exited the oral area. The highest values were located in the mouth area and they were a magnitude higher than in comparison to the values in the nasal cavity. This was expected as the mouth was considered the inlet. The obtained maximum value can be compared to the value obtained in paper [43], although the location is different due to the difference in the inlet geometry.

For the nose inlet, the turbulent kinetic energy decreased as the airflow exited the pharynx, compared to the oral area in the previous case. In this case, the values were a magnitude higher compared with the mouth inlet.

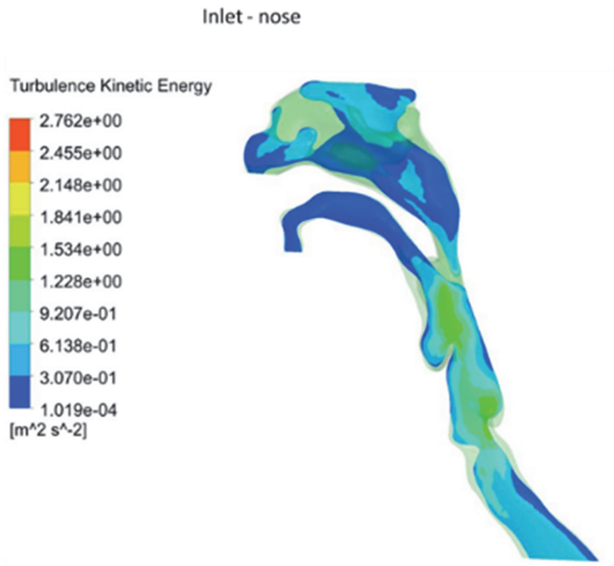

Figure 8 Turbulence kinetic energy for the nose inlet

The shear stress distribution can be useful for the healing of the epithelial lining of the lungs. This parameter can be very useful considering air pollution and the effect that air pollutants have on the respiratory and cardiovascular systems. The shear stress values can be seen in Fig. 9.

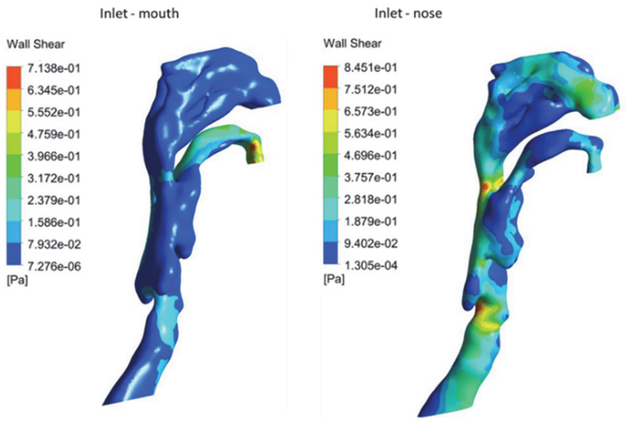

Figure 9 Shear stress values

As it can be seen in the figure above, the maximum shear stress values were 0.71 Pa and 0.85 Pa for simulations where the inlet was mouth and nose, respectively. In the case of the mouth inlet, the highest values were calculated in the oral area, while in the case of the nose inlet the highest values were calculated in the pharynx area.

3.2 Particle Tracking

The flow patterns can be used to provide information regarding potential deposition locations. Considering that particle movement depended on the airflow, information regarding the highest velocities could be useful to determine potential deposition locations. Based on this, for the mouth inlet, the particles were expected to deposit close to the inlet, while for the nose inlet, the particles were expected to deposit in the pharynx and larynx segments.

The comparison of the particle tracking in the upper respiratory tract when air and particles were inhaled through the mouth and nose can be seen in Fig. 10. Considering that only the short period of time of the breathing cycle was considered (0-2.5 s), these results can be considered as the initial prediction of particle location in the upper respiratory tract during the inhalation part of the breathing. The type of inlet had a significant effect on particle tracking. The number of particles considered for the nose inlet was double the amount of particles for the mouth inlet. The reason for this was the area of both inlets, as the nose inlet consisted of two openings, each similarly sized to the mouth inlet. Taking that into consideration we chose to double to amount of particles injected into the nose. For the mouth inlet, particle deposition was close to the inlet, as predicted by the highest velocities. For the nose inlet, obtained particle deposition cannot be completely compared to the highest velocity location, as in this case particles were mostly deposited in the nasal cavity.

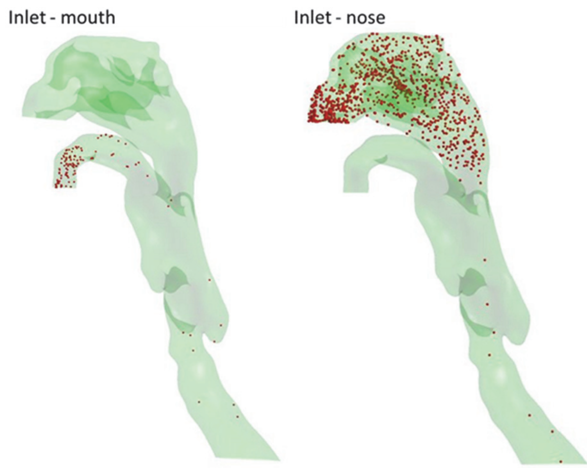

Figure 10 Particle depositions for the mouth and nose inlet

The obtained results for particle deposition for the mouth inlet can also be compared to the results of the shear stress for the same inlet. As it can be seen by comparing these two figures, the highest amount of particles was located in the area where the shear stress was the highest. However, when considering the nose inlet it cannot be compared.

Particles deposited in the respiratory system can lead to tissue inflammation and as a result cause different health problems. Inflammation leads to damage of the respiratory tract cells and endangers the integrity of the respiratory system. The presented approach can be useful for reducing the number of examination procedures clinicians need to perform. However, this is still considered to be an innovative approach. In order to be able to employ this approach in medicine, a developed model needs to have an accurate prediction of particle deposition. The only way to validate particle prediction in a respiratory system requires to expose a patient to inhaling drugs that have been radiolabeled. Although we are able to perform very complex simulations, the validation process keeps this from being widely employed by clinicians for individualized patient treatment.

4 CONCLUSION

The obtained simulation results of airflow and particle deposition for two types of inlets (mouth and nose) were presented. Analysis of the airflow field using CFD analysis provided information about velocity, turbulent kinetic energy, shear stress, and pressure during the inhalation segment of the breathing cycle. Based on the obtained airflow field, location and particle deposition were analyzed. For mouth and nose inlets, the majority of particles were deposited in the mouth and the nasal canal, respectively. Results presented using the CFD-DPM approach were obtained with several simplifications in order to reduce the need for computational resources.

Future work will include improved mouth inlet as well as the new simulations with additional types of pollutants. Also, the presented model did not include particle interactions, which will be considered in future studies.

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