

Computational Fluid Dynamics-Based Respirator Fit Evaluation - A Pilot Study

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ABSTRACT

This paper presents a computational fluid dynamics (CFD)-based approach to evaluate fit of a filtering facepiece respirator (FFR). A medium size digital headform and a medium digital FFR were obtained from the National Institute for Occupational Safety and Health (NIOSH) database. After the headform and the FFR contact was simulated, a chamber was generated to represent the zones of the FFR cavity, the filtering medium and the region outside the FFR. Inside the chamber, air flow and particle movement were calculated. The air flow was driven by the human inhalation and the freestream towards the human face, and the particle movements were driven by the air drag force and gravity force. Respirator fit was evaluated by a computer simulated fit factor (CSFF) defined as the particle concentration of the air flow inhaled by the nostril to the particle concentration of the air flow passing through the flow inlet boundary. The CSFF of the headform/FFR combination in the simulation results was 90.20, which was higher than 10, the Assigned Protection Factor for FFRs and was lower than 150-200, which encompasses most of the fit factors measured in experiments. The simulation results also showed that the geometries of the human face and FFR affected the air flow pattern in the region outside FFR. The air flow velocity inside the FFR cavity was distinctly different from the velocity outside. The particles inside the FFR cavity were not uniformly distributed.

Keywords: Computational fluid dynamics, filtering facepiece respirator, particle movement, respirator protection factor.

INTRODUCTION

Respirators play an important role in protecting workers from harmful particulates, fumes, vapors, etc. Fit factor is critical for respirator users, designers and manufacturers, and quality monitoring agencies. The OSHA respiratory protection regulation defines the standard eight-exercise procedure in respirator fit tests (OSHA, 1999). The particle concentration inside the respirator cavity (C_{in}) is calculated through dividing the total mass of particles inside the cavity by the volume of the cavity. Similarly, the particle concentration outside the respirator (C_{out}) can also be calculated. The fit factor is the ratio of C_{out} to C_{in} . The respirator fit factors must be determined experimentally according to current regulation. However, the experimental approach is time consuming and expensive. A computational filtering facepiece respirator (FFR) has been constructed as the computational model that has the same shape of the FFR and the function of filtering particles. This pilot study was to investigate a novel computational fluid dynamics (CFD)-based method to predict the fit factor for computational FFR.

The quantitative fit test has been performed on respirator users for characterizing the respirator sealing ability. The respirator fit test includes a series of exercises that are performed by the subject. The fit factor is defined as the ratio of the concentrations of challenge aerosol outside the respirator to the concentrations in the respirator cavity during the fit test. The TSI Fit-Test Probe Kit (P/N 8025-N95, TSI, Shoreview, MN, U.S.A.) has been widely used for generating the ambient aerosol, measuring the particle concentrations and calculating fit factors (Coffey et al., 1999; 2002). The fit factor of N95 FFR is directly related to the proportion of ambient particles entering inside the N95 FFR cavity. The particle pathways are through the face seal leakage and through the filtering medium, of which most of the particles enter the N95 FFR cavity through the imperfect face seal (Grinshpun et al., 2009). It was reported that the filtration efficiency of the N95 respirator increases with particle size and reaches above 99.5% at about 0.75 μm of particle size when no face seal leakage occurs (Qian et al., 1998).

Zhuang et al. (2005) studied the effect of subject facial characteristics on respirator fit and recommended measurements of face length and face width for defining the panel for N95 FFR. Two panels for fit testing respirators, including one based on face length and face width and the other one based on principal component analysis of facial dimensions, were developed by National Institute for Occupational Safety and Health (NIOSH) researchers (Zhuang and Bradtmiller, 2005; Zhuang et al., 2007). A correlation was found between the face sizes and the respirator fit (Zhuang et al., 2008).

Lagrangian particle tracking was used to model indoor airborne particles, particle interaction with human breathing and deposition in a human nasal cavity geometry (Zhang and Chen, 2006; Zhang and Chen, 2007; Se et al., 2010; Li et al., 2012). By simulating indoor particle movement, Anthony and Flynn (2006) and Anthony (2010) found that particle diameter and breathing velocity significantly influenced the particle size distribution. Li et al. (2005) provided a mathematical model for investigating the mechanism of virus transfer in a facemask during breathing. The viruses' movement outside of the filtering medium was not considered in the model. This model contains several coupled systems, and is difficult to construct using CFD simulations, especially in 3D simulation with a complicated geometry. To the authors' knowledge no one has investigated the 3D CFD simulation of particles moving in a FFR cavity.

In our previous research, the FFR-headform contact, especially the contact pressure and contact area, were studied by both experimental and computational methods (Lei et al., 2011; Lei et al., 2013a). The contact simulation provided the accurate assembling of the FFR and the headform, when they contacted each other and deformed. By using the CFD method, the heat transfer and breathing air flow between the contacted headform and FFR were simulated for the study of FFR leakage (Lei et al., 2013b). In this study, a chamber was generated to represent the zones of the FFR cavity, the filtering medium and the region outside the FFR. Inside the chamber, air flow and particle movement were calculated. The objective of this paper was to investigate a simulation-based approach to predict FFR fit factor.

METHODS

The numerical model involved the surface contact, the air flow and the particle movement. The finite element (FE) contact simulation determined the geometries of the FFR and headform when they contact each other. The CFD simulation calculated the air flow and particle movement for the FFR fit factor prediction.

FE Contact Simulation

This CFD-based study utilized the medium size headform developed by NIOSH, as well as a digital model of FFR (3M 8210) that was scanned by NIOSH using a 3D imaging system. The FE

headform was constructed from its scanned models using the method developed by Lei et al. (2010; 2011). The headform model consisted of six regions: forehead, left cheek, right cheek, chin, neck, and back of the head, and had layers of skin, fatty tissue, muscle and bone. The facepiece of the FFR FE model was obtained using the scanned data. The two straps were modeled based on the measurements of the lengths and widths of the straps. An adjustable nose clip, defined as plastic metal material, was also modeled in the FFR model.

The entire contact simulation process had three steps. The first step was to pull the straps around the back of the headform and to pull the FFR away from the face. The second step was to attach the straps to the FFR and to release the FFR so that it moves towards the face. The third step was to deform the nose clip for molding the nose area to the shape of the nasal bridge. In its final state, the FFR contacted the human face. We assumed that the headform remained static during the FFR contact.

CFD Simulation

A coupled effort of the air flow and the particle transport around the face of the headform was solved to predict the FFR fit factor by the open source CFD software, OPENFOAM 2.10 (OpenCFD Ltd., ESI Group, Bracknell, UK). Originally, all particles were located outside of the FFR. Then, because of the air flow and occurrences of leak locations, particles were able to move into the FFR cavity and eventually entered the human respiratory system. The sources of air flow came from the human respiration and environmental freestream flow. Thus, the air flow field should include three zones: between the headform and the FFR, inside the FFR medium and outside of the FFR. The CFD simulation method consisted of three components: generating the meshed zones of the air flow field, defining the mathematical model, and designing a numerical scheme to calculate the air flow and particle movement.

The headform and FFR surfaces from the FE contact simulation were used to generate meshes for the air flow field. Fig. 1(a) presents the inner surface of the FFR and the outer surface of the headform that were extracted from the final state of the contact simulation. The headform surface was trimmed for computational efficiency, as shown in Fig. 1(b). A MATLAB program was developed to create meshes and to export the meshes to the file that can be read by the OPENFOAM software.

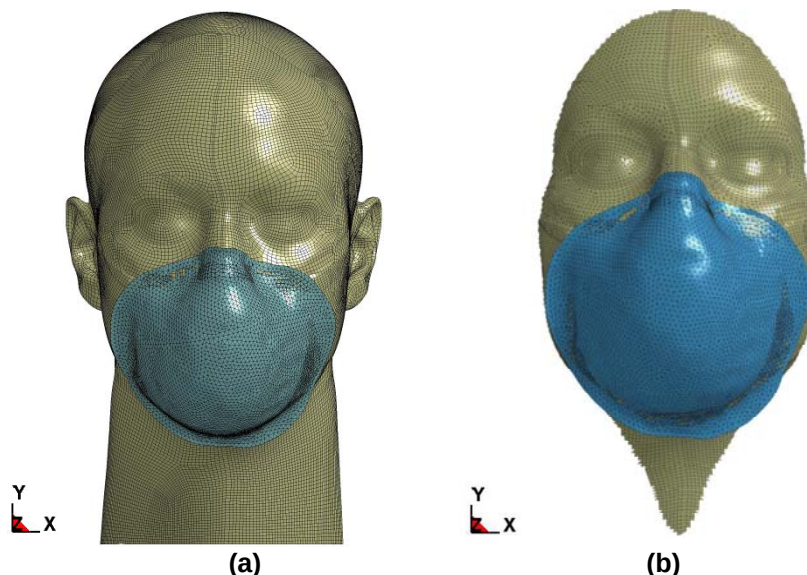


Fig. 1: (a) The inner surface of the FFR and the outer surface of the headform; (b) the inner surface of the FFR and the trimmed surface of the headform.

The geometry was meshed into three zones: Zone I (the FFR cavity), Zone II (the FFR filtering medium) and Zone III (outside of the FFR), as shown in Fig. 2. The maximum dimension of the whole meshed domain in the z axial direction was 160 mm . Zone I consisted of five layers of elements, which had the same thickness at the arbitrary location with the same x and y coordinates. Zone II had one layer of elements with a uniform thickness of 3 mm , the thickness of the FFR filtering medium. Zone III had a structure of twenty-six layers with 6 boundary layers and a structure of twenty layers without 6 boundary layers. The six boundary layers had a thickness of 0.5 mm and other layers in Zone III had the thickness of 7.7 mm .

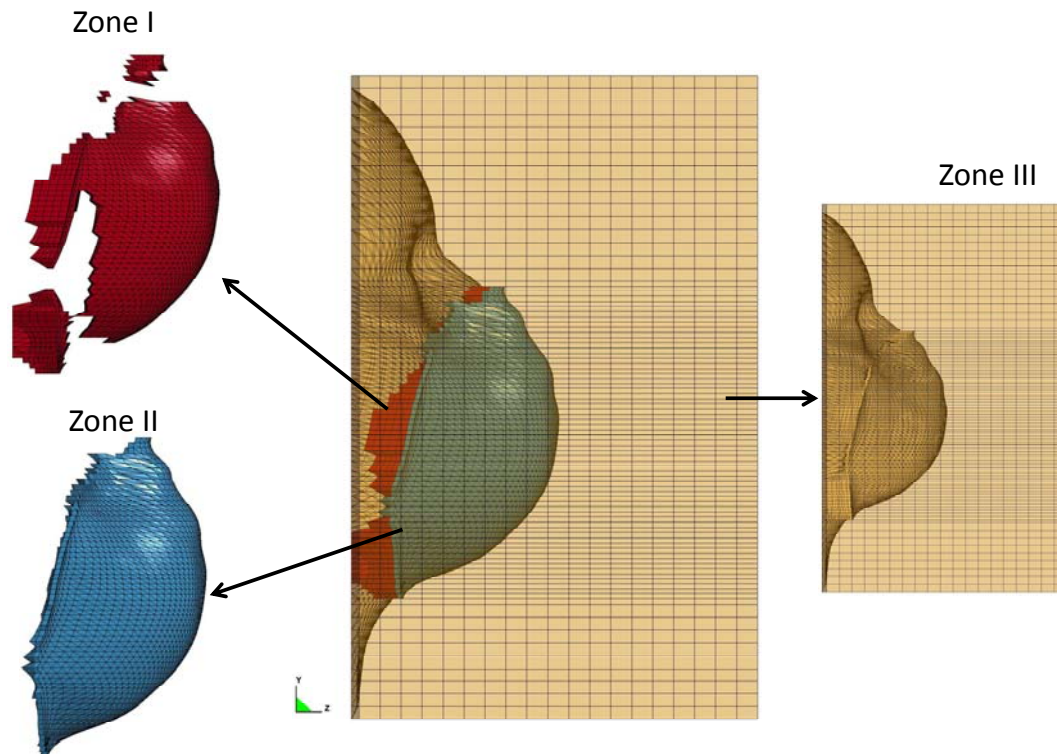


Fig. 2: Mesh generation in Zone I (the FFR cavity), Zone II (the FFR filtering medium) and Zone III (outside of the FFR).

The external surfaces of the entire computational domain were defined with five boundaries: the nostril, human face, exterior I&II, and flow inlet, as shown in Fig. 3. Since our problem only included the normal breathing with a low respiratory flow rate, we assumed that the respiration in this study was purely nasal breathing. The nostril was considered as a square with about 1 cm^2 area, determined by the scanned nasal geometry of the headform. In our previous study for determining the leak locations of FFR-headform, the periodic change of the exhalation and inhalation was implemented by defining an unsteady mass flow rate at the boundary of human nose. The current study, however, focused on how particles enter the human respiratory system and we assumed that the breathing pattern only contained the inhalation. Based on the normal breathing pattern of a human subject who donned a respirator (Grinshpun et al., 2010), the velocity with a magnitude of 1.51 m/s and the direction towards the nostril was assigned to the human nose boundary. The freestream velocity with the magnitude of 1 m/s and the $-z$ axial direction (towards human face) were defined at the velocity inlet. We assumed that there was neither head movement nor no FFR deformation during the CFD simulation. The boundary of human face was defined as a non-slip boundary condition with zero velocity. The exterior I & II have the pressure outlet boundary condition, in which the air velocity was unknown, but the pressure was equal to the

standard atmospheric pressure (the gauge pressure is 0 Pa). At the initial time, the internal flow field had a uniform zero velocity and a uniform zero gauge pressure (0 Pa).

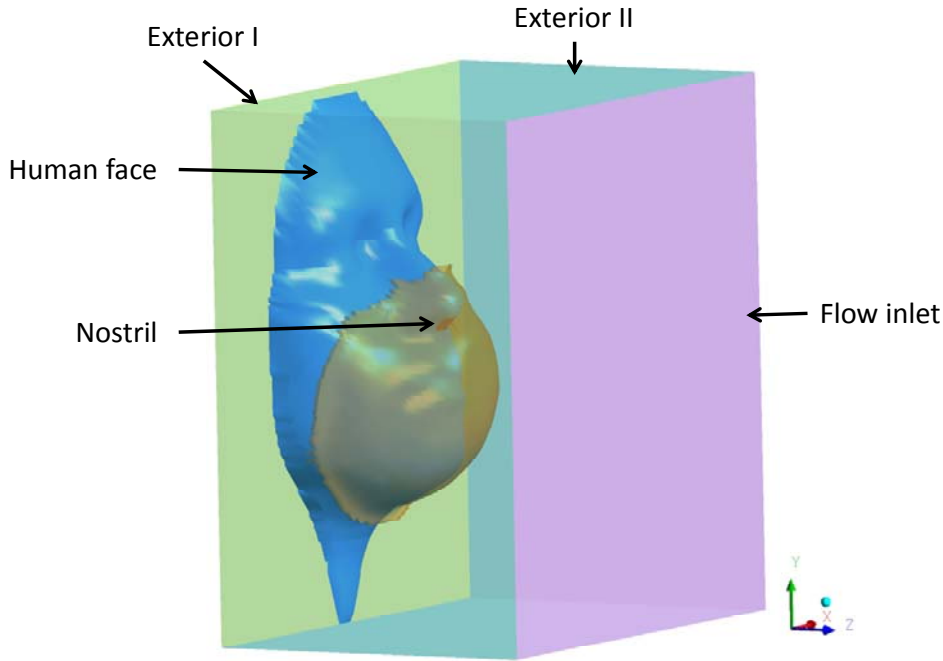


Fig. 3: Boundary conditions.

The mathematical model of the air flow included governing equations for three flow zones, boundary conditions and initial conditions. We assumed that the fluid in both Zone I (FFR cavity) and III (outside of the FFR) was dry air and ignored the impact of the water vapor, CO₂ and temperature. Additionally, Zone I and III were directly linked by small leak gaps that came from the imperfect facial seal on the FFR's border. Thus, the air flow in Zone I and III can be described by mass conservation and momentum conservation equations. The standard k-epsilon model, which introduced a turbulent kinetic energy term k and a turbulent dissipation term ε was selected for describing the turbulence. Zone II (FFR filtering medium) that was made up of randomly-oriented fibers can be defined as a porous media in order to simulate its resistance to flow. The air flow inside the N95 FFR filtering medium was described by Darcy's law, represented by Eq. (1).

$$\nabla p_a = -\mu_a D \mathbf{V}_a \quad (1)$$

where p_a was the air pressure, μ_a was the air viscous coefficient, D was the viscous resistance coefficient and $\mathbf{V}_a$ was the air velocity vector (Brinkman, 1949; Li et al., 2005). A viscous resistance coefficient, $D = 1.12 \times 10^{10} (m^{-2})$, was adopted for the FFR layer based on experiments quantifying the air permeability of FFRs (Li et al., 2006).

In the Lagrangian frame, a particle was established by giving the position of its center $\mathbf{X}_p$, its diameter D_p , its velocity $\mathbf{V}_p$ and its density ρ_p . Newton's equation, represented by Eq. (2), was used to govern the motion of the particle.

$$m_p \frac{d\mathbf{V}_p}{dt} = \mathbf{F}_D + m_p \mathbf{g} \quad (2)$$

where m_p was the mass of the particle calculated by $m_p = 1/6 \rho_p \pi D_p^3$, $\mathbf{V}_p$ was the particle velocity,

$\mathbf{F}_D$ was the drag force from the air flow, and $m_p \mathbf{g}$ was the gravity force. When the air flow passes the filtering medium, the air drag force could push particles to impact the filtering medium surface. The particles could not penetrate the filtering medium. The OPENFOAM software has a well design solver for simulating particle movements in Lagrangian frame. In each time step, after the air flow field, including the velocity, pressure, turbulent kinetic energy and a turbulent dissipation, were calculated, velocities and positions of particles were updated.

We assumed that particles in a simulation were in the same size $1 \mu\text{m}$. For each time step (0.001 s) on the flow inlet boundary, 1000 particles were injected into the domain with an initial velocity of 1 m/s in the $-z$ axial direction. The impact between airborne particles and the FFR filtering medium was considered in the simulation. Qian et al. (1998) reported that an N95 FFR can filter 99.5% of particles, if the particle size is larger than $0.75 \mu\text{m}$. We assumed that no particle can enter FFR cavity through FFR filtering medium. As an implementation of OPENFOAM's solver, we defined a function that monitored the impact between a particle and the FFR filtering medium. In order to simulate the process that FFR filtered airborne particles, after the particle impacted the filtering medium, the particle stuck to the filtering medium and its velocity remained zero in the rest of the simulation.

The algorithm named Semi-Implicit Method for Pressure-Linked Equation (SIMPLE) was selected. The second-order upwind scheme was used for the velocity, pressure, turbulent kinetic energy and turbulent dissipation, since it is more accurate in unstructured grids. Duration of 1 s was simulated with a time step 0.001 s. In each time step, numerical iterations were performed until the residuals of continuity, x-, y- and z-velocity, pressure, turbulent kinetic energy and turbulent dissipation were below 1×10^{-5} which indicated a convergent solution.

Computer simulated fit factor (CSFF) was defined as the particle concentration of the air flow inhaled by the nostril ($C_{inhaled}$) to the particle concentration of the air flow passing through the flow inlet boundary (C_{inlet}):

$$CSFF = \frac{C_{inhaled}}{C_{inlet}} \quad (3)$$

The CSFF was determined during $t=0.5-1.0$ s. The particle concentration of the air flow through the nostril ($C_{inhaled}$) in this time period was calculated as the ratio of the particle number to the flow volume. Similarly, C_{inlet} in this time period was calculated.

RESULTS

Fig. 4(a) shows, at $t=1$ s, the velocity vector field, the velocity contour at the sagittal plane, and the air flow streamlines backward from the nostril. Velocity vectors of the air flow that were thoroughly distributed within the whole domain indicated a fully developed flow pattern. The velocity vector field also showed that the air flow had the trend of following the geometrical features of the human face and FFR when it was near the human face. The air velocity contour in Fig. 4(b) showed that in the FFR cavity the air velocity (about 0.3 m/s) was distinctly lower than the air velocity at the region far from the respirator (about 1.0 m/s). The FFR filtering medium reduced the air flow velocity. The air flow streamlines in Fig. 4(c) showed that the air flow entered the FFR cavity through the FFR filtering medium and the leak

locations (on the cheek). The majority inhaling air streamlines passed through the region of filtering medium about 20 mm below the nostril.

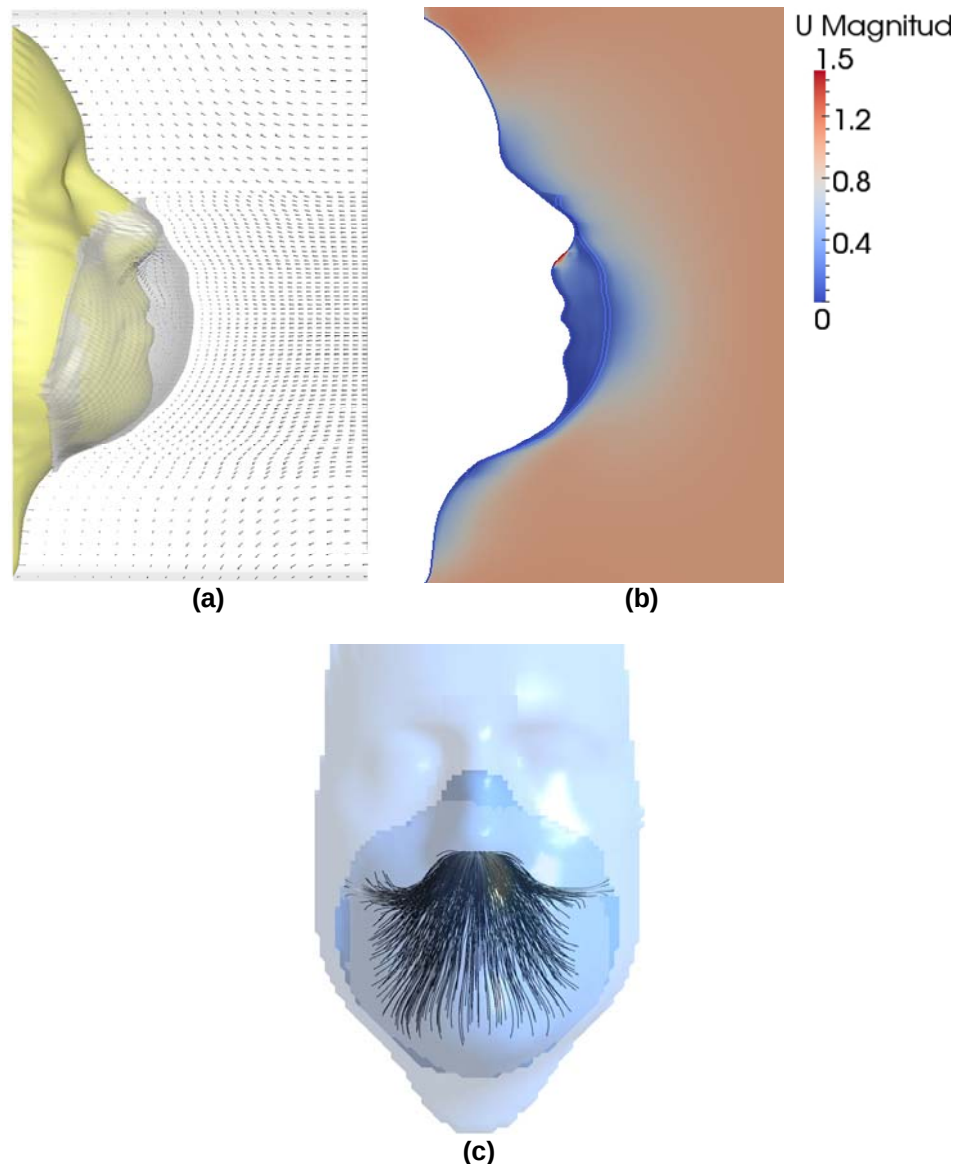


Fig. 4: CFD simulation: (a) The air velocity vector field in the domain at $t=1$ s; (b) the air velocity contour on the sagittal plane at $t=1$ s; (c) the streamlines of air flow in the domain at $t=1$ s.

Fig. 5(a) shows the particle distribution in the whole domain. Fig. 5(b) shows the particle distribution inside the cavity by clipping the whole domain using the y-z plane into a 20 mm layer ranging from $x=-10$ mm to $x=10$ mm. The internal cavity had a much lower particle concentration than the external environment. Particles were not uniformly distributed inside the FFR cavity and most of them were located at the region below the nostril and near the leak locations that were the left and right cheeks. The CSFF calculated for the time period $t=0.5-1.0$ s was 90.20, which was higher than the Assigned Protection Factor for FFRs 10 (OSHA, 2006; 2009; Ronald and Rengasamy, 2009) and was lower than most of the fit factors measured in experiments 150-200 (Roberge et al., 2011).

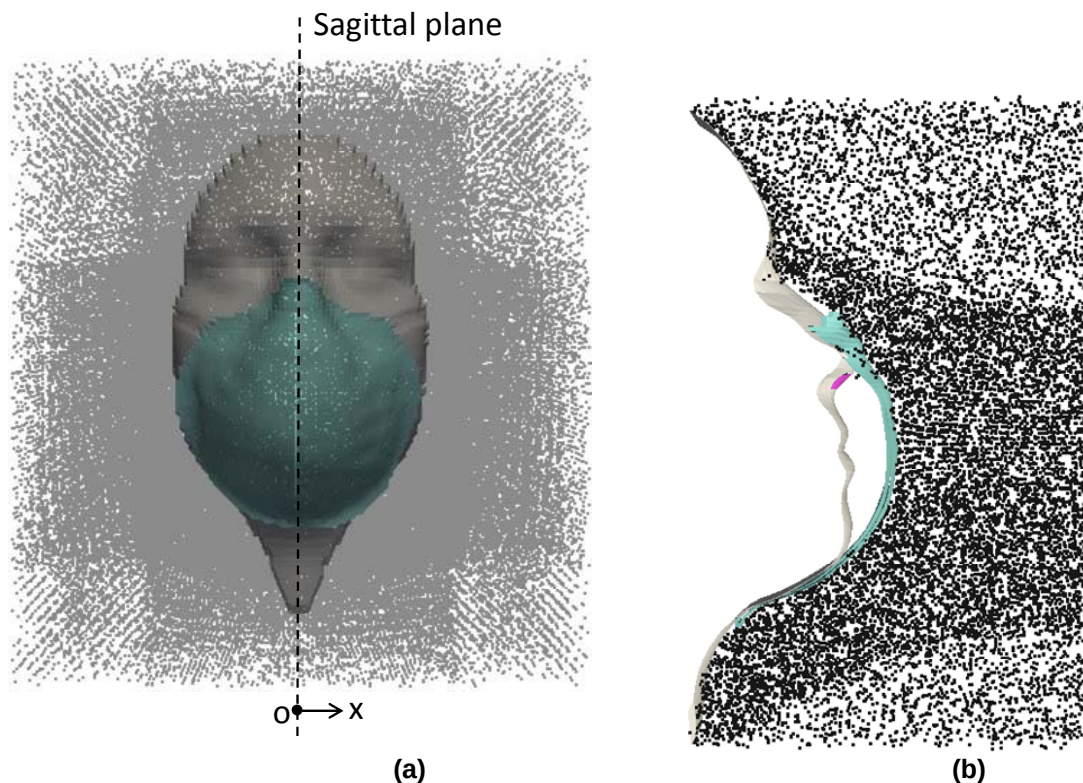


Fig. 5: The particle distribution (a) in the whole domain, frontal view; (b) in the clipped domain from $x = -10 - +10$ mm, in which the grey color region is the human face, the pink color region is the nostril, the blue color region is the N95 FFR filtering medium, and the black color points are the particle.

DISCUSSION

The results showed that the air flow outside of the FFR was affected by the freestream flow and the headform-FFR geometry. It was also shown that the flow and particle movement inside the FFR was impacted by the inhaling air flow. The streamline pattern inside the cavity represented the air flow pattern that was difficult to be captured by experimental approach. The advantage of our CFD-based method is that it can provide more information on the external and internal air flow characteristics and particle movement. Another advantage is that the simulation is safe in the application of studying the dangerous agent, like the virus particle. Moreover, to change the parameters, including the particle size, the breathing pattern, the freestream flow and the leak size and location, in the simulations is easier than to change them in the experiments. In the future study, we will investigate how these parameters affect the respirator fit factor.

In respirator fit test for measuring fit factor, a sample probe is inserted into the respirator cavity. The probed concentrations inside the respirator cavity were found to have large measurement error and to be related to the location and depth of the sample probe (Bergman et al., 2013). The simulation results in this study showed that the particles were not evenly distributed inside the cavity. Hence, different probing locations provided difference particle concentrations. Instead of determined the particle

concentration inside the FFR cavity we calculated the particle concentration of the air flow through the nostril, which directly indicated the amount of particle entering human respiratory system.

The limitations of the simulation results came from several simplifications in this study. First, we used purely inhalation as the respiratory pattern and the role of exhalation on fit factor was ignored. The exhaled air flow can lower the particle concentration inside the FFR cavity. Second, the traditional fit test requires the subject to perform several exercises. The exercises may affect the particle concentration inside the FFR cavity. Although the exercise of deep breathing can easily be added into our simulation, the exercises of head movements and facial expressions require further investigation. Third, we considered the large size particles ($1\ \mu\text{m}$) and assume that the particles were not able to pass through the filtering medium. However, researchers have found that small size particles (nanoparticle) have a higher penetration rate through the filtering medium (Shaffer and Rengasamy, 2009). Fourth, the impact of the particle diffusion was not considered in this computational model. Future work will add the diffusion model into the simulation. Fifth, the simulation results were not validated by experimental results.

CONCLUSIONS

The novelty of this study was to investigate an alternative approach to evaluate respirator fit as compared to traditional experimental fit tests. The air flow field inside the FFR cavity, the flow through the FFR filtering medium and the freestream flow outside were simulated by our proposed CFD-based method. In addition, the particle movements, driven by the air drag force and gravity force, were calculated for determining the CSFF. The simulation method is a promising method to easily and safely check the cause and effect.

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