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Accurate CFD prediction of respiratory airflow and dispersion through face mask

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Abstract. This study develops an accurate modelling framework of flow and dispersion through face mask based on computational fluid dynamics (CFD) theory and method. The influence of gird division, time step size, and turbulence model on simulation accuracy were investigated. The result shows that the viscous resistance coefficient and inertial resistance coefficient of face masks (surgical masks) were 3.65×10^9 and 1.69×10^6, respectively. The cell size on the surface of face masks should not be larger than 1.0 mm; the height of the first layer cells near the face masks should not be larger than 0.1 mm; and the time step sizes discretizing the breathing and coughing periods should not be more than 0.01 s and 0.001 s, respectively. The results given by LES model show closer agreement with the experimental data than RANS models, with approximately 10% relative deviation for the air speed near the face mask. Overall, the SST k-ω model performs the best among the RANS models, especially for the air speed. The findings obtained form a CFD modelling framework for an accurate prediction of airflow and dispersion problems involving face masks.

1. Introduction

Statistics show that the COVID-19 pandemic could result in a monthly global consumption and waste of 129 billion face masks. In addition, even during the non-pandemic period, face masks are the basic consumables of hospitals. However, the performance of face mask, in terms of protective efficacy and negative health effect to users, has not been well understood. As one of common evaluation methods, experimental measurement has usually been adopted in the study of face masks. However, it is difficult for experimental methods to measure accurately the respiratory airflow and dispersion through a face mask. Alternatively, numerical simulation is an important method to increase the understanding of the health effect of face masks and to develop high-performance ones. However, the accuracy of CFD technology depends largely on the user's knowledge of fluid dynamics and the experience and skills of using numerical technology, specifically and particularly being influenced by the selection of turbulence model, time step size, grid generation, and boundary conditions etc. There is so far no an accurate modelling framework of flow and dispersion through face mask based on CFD theory and method. This study aims to address this problem. The value and significance of this study is to establish a modelling framework for accurate CFD prediction of face masks under using status and in turn to promote further studies and improvements on face masks and other face shield technologies.

2. Methodology

Methodology includes the following four parts. First, the filtering performance of commonly used surgical masks was experimentally tested to obtain the boundary conditions for CFD simulations. Then, the air speed and concentration through the face mask when its user is breathing and coughing were measured via human subject experiments, so as to validate CFD modelling framework. Finally, based on the porous media model, the influence of turbulence model, grid distribution, and time step size on

the simulation accuracy of respiratory airflow and dispersion through face mask under different expiratory activities (breathing/coughing) was investigated. The computational geometry and boundary conditions are described as follows and other parts of methodology are omitted.

A full-scale test room with dimensions of 4 m-length × 3 m-width × 2.6 m-height was employed. The floor, ceiling, and walls around the room were set to be no-slip, stationary, and adiabatic, with the internal emissivity to be 0.95. The ventilation mode of the room was mixed ventilation, where an air inlet with dimensions of 0.4 m-length × 0.2 m-height was located at the bottom of the side wall and an air outlet with the same dimensions was located at the top of the same side wall, as shown in Figure 1. A 3D computational thermal manikin (CTM) wearing a face mask, with a height of 1.72 m and a total surface area of 1.66 m^2, was located in the middle of the room and facing the wall with air inlet and outlet.

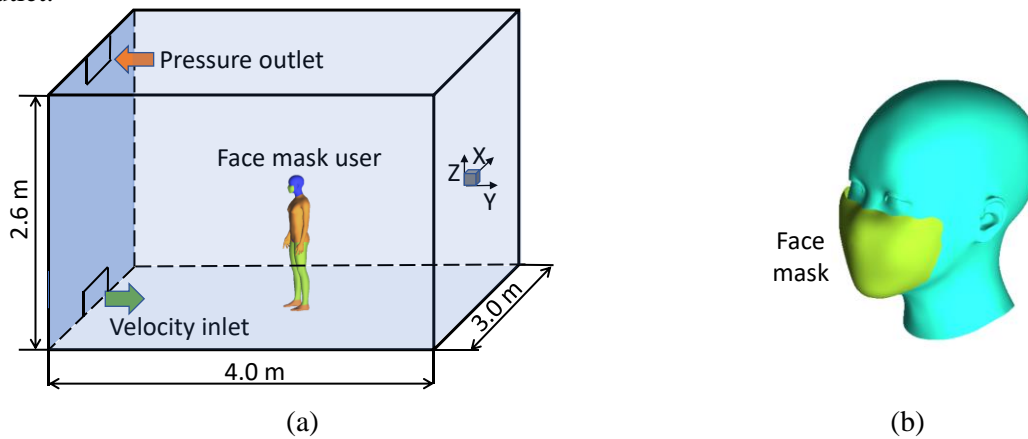(a)   (b)

Figure 1. Geometrical model: (a) test room and (b) human head wearing a face mask.

In the present study, the surface of the CTM was divided into different parts with different skin temperatures, and detailed information can be found in our previous study. In addition, the heat transfer between human body and surrounding air through both convection and radiation was considered. According to the study by Murakami et al., the internal emissivity of human skin was defined as 0.98. Two typical expiratory activities including breathing and coughing were investigated. The airflow patterns under different expiratory activities are shown in Figure 2. During normal breathing, the opening area of mouth was about 120 ± 52 mm^2, but exceeded 400 ± 95 mm^2 during coughing. Hence, the mouth opening area was defined to be 132 mm^2 and 360 mm^2 for breathing and coughing, respectively. In the breathing process, the pulmonary ventilation rate was set to be 9 L/min, representing light-level activities in sitting and standing postures. The exhaled air and ambient air were considered as incompressible ideal gas to simulate buoyancy effect. The tracer gas, carbon dioxide (CO_2) widely representing the exhaled pollutants, was released from the mouth with a fraction of 4.5%.
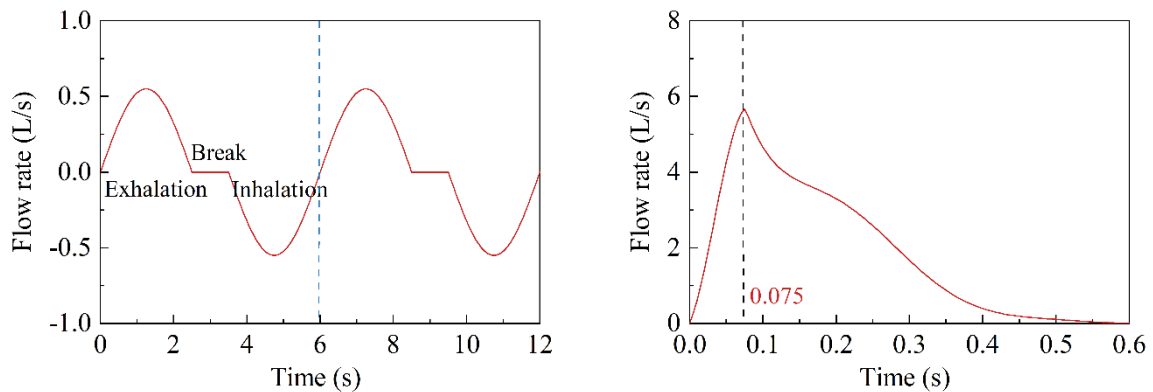
Figure 2. Airflow patterns under different expiratory activities: (a) breathing and (b) coughing.

The lace of face mask was omitted in the simulations. In order to make the face mask fit the face perfectly, the shape of face mask has to be adjusted when wearing in practice. In the present study, a geometrical model of face mask was developed according to the adjusted shape under using status. The thickness of the face mask was set to be 1.0 mm based on the present measurement and those reported in previous studies, namely, 0.5-2.3 mm, depending on the type of face mask. It was reported that the gap size between the face mask and face was around 4-14 mm, influenced by the wearer's face shape and wearing habits. In the present study, the largest gap size was less than 10.0 mm, which was located on the top of face masks. Overall, the geometrical model of face mask developed in the present study is close to the reality.

3. Conclusions
The findings from the present study allow the following conclusions to be drawn.
(1)   The boundary conditions of surgical masks required by the porous media model were determined by experimental test and mathematical fitting, where the viscous resistance coefficient and the inertial resistance coefficient are 3.79×10^9 and 1.69×10^6, respectively.
(2)   The cell size on the surface of face masks should not be larger than 1.0 mm, and the height of the first layer cells near the face mask should not be higher than 0.1 mm.
(3)   The time step sizes discretizing the breathing and coughing periods are better to be kept no more than 0.01 s and 0.001 s, respectively.
(4)   The LES model is more accurate than RANS models in predicting respiratory airflow and dispersion through face mask, with approximately 10% relative discrepancies for the air speed near the face mask from the experimental data.
(5)   Compared with LES model, the SST k-ω model performs best among the RANS models, especially for air speed, with 5.1-20% relative deviation.

References
[1] Jia Z J, Ai Z T, Yang X H and Mak C M 2022 Towards an accurate CFD prediction of airflow and dispersion through face mask Build. Environ. Accepted.