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Towards an accurate CFD prediction of airflow and dispersion through face mask

A B S T R A C T

Given the difficulty of experimental measurement of respiratory airflow and dispersion through a face mask, accurate numerical simulation is an important method to increase the understanding of the health effect of face masks and to develop high-performance ones. The objective of this study is to develop such an accurate modeling framework based on computational fluid dynamics (CFD) theory and method. For model validation, the flow characteristics through the face mask were tested experimentally, and the air speed and exhaled pollutant concentration in the breathing zone were measured with human subjects. 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 × 109 and 1.69 × 106, 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 modeling framework for an accurate prediction of airflow and dispersion problems involving face masks.

Keywords: Face mask; Computational settings; Turbulence model; Respiratory airflow and dispersion; CFD simulation.

1. Introduction

Up to September 2022, the coronavirus disease of 2019 (COVID-19) has caused more than 600 million confirmed cases and 6 million deaths [1]. As one of the high-efficiency and low-cost prevention measures for pandemic, wearing face masks is extensively recommended by the World Health Organization (WHO) and the US Centers for Disease Control and Prevention (CDC). A study shows that the pandemic could result in a monthly global consumption and waste of 129 billion face masks [2]. In addition, even during the non-pandemic period, face masks are also the basic consumables of hospitals.

Protective efficacy of the face mask has been widely discussed. On one hand, filtration characteristics of face masks, including breathability [3,4] and particle removal efficiency [3], vary across different materials. On the other hand, the protective efficacy of face masks in wearing process was studied through manikin/subject experiment [5,6]. The long-term wearing of face masks especially for medical staffs has brought some negative effects including skin damage [7], headache [8], hypoxia [9] and discomfort [10]. Sukul et al. observed a significant and consistent decrease in peripheral oxygen saturation and an increase in partial CO2 pressure, which are most pronounced for elderly subjects and in the conditions with the use of FFP2 masks [9]. An accurate understanding of the protective efficacy of face mask and its negative effect is the basis of developing face masks with high-protection efficiency and low-negative health effect.

As one of common evaluation methods, experimental measurement has usually been adopted in the study of face masks. The particle concentration in front of the face mask and the exhaled air leakage at the side of the face mask should be measured to evaluate its protective efficiency. The microenvironment inside the face masks (includingconcentration, speed, air temperature, humidity, etc.) should be measured to evaluate the effect of face mask on the thermal comfort and the inhalation exposure of self-exhaled pollutants. However, there are three obstacles to the accurate evaluation of face masks by experimental methods. First, for the internal microenvironment covered by a face mask, the relatively closed space makes it difficult to arrange measurements. In addition, airflow and concentrations with intense fluctuation and instantaneity due to human expiratory activities require that the time constants of measuring instruments must be short enough to record the details [11]. Second, different gap sizes existed around the different edges of face masks would lead to different leakage rates [12, 13], especially at the top, bottom, and side edges of face mask [14–16]. However, the experimental measurements often provide only limited data at discrete measurement locations. Hence, an accurate evaluation on the amount of air leakage from face mask edges is almost impossible. Third, the air speed after penetrating through a face mask decays rapidly to less than 0.3 m/s [17], with nonuniform distribution, also making the experimental evaluation of the protective efficacy of a face mask rather difficult.

Compared with experimental measurements, computational fluid dynamics (CFD) technology provides richer details, higher flexibility, and lower cost [18], and expediently performs parameter analysis to examine the role of specific parameter in the whole system. Hence, CFD technology can overcome the above obstacles encountered during the experimental measurements. 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 [18], specifically and particularly being influenced by the selection of turbulence model, time step size, grid generation, and boundary conditions etc. [19,20].

Among above mentioned influencing factors, the turbulence modeling method is a key directly affecting the CFD simulation accuracy and efficiency [18]. The turbulence models that have been adopted to face mask/shield simulations mainly include RANS method and LES method, as shown in Table 1. At present, the selection of turbulence model in most studies on face masks are based on the previous experience obtained from the studies on conventional indoor airflow and dispersion problems. However, the airflow and dispersion around a face mask under using status are quite different from indoor problems in terms of spatial and time scales. The narrow space enclosed by face mask and face is obviously smaller than the room scale. The exhaled air with large momentum enters this space causes more intense turbulence with smaller scales. In addition, the periodic expiratory activities [21,22] with short durations [23] make the airflow and dispersion different from the time scales of those of the room. Therefore, it is necessary to evaluate the adaptability and suitability of turbulence models in the simulation of face masks.

The temporal and spatial discretization is important process of CFD simulation, which largely determines the numerical accuracy and computational cost. In order to capture the flow characteristics of exhaled air, a small enough time step size is required. A review of the time step sizes adopted to CFD simulation of human expiratory activities is shown in Fig. 1. The time scales required for the temporal resolution of different expiratory activities are obviously not the same, which are still unclear so far. In addition, the grid distribution on and around face masks represents the most refined spatial scales, which determines largely the number of cells in the whole flow field and thus the computational cost and accuracy. Overall, the suitable temporal and spatial discretization regarding the CFD simulation of face mask is worthy of further exploration.

This study aims to address the aforementioned problems associated with the accurate CFD prediction of airflow and dispersion around a face mask under using status. 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 modeling 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 value and significance of this study is to establish a modeling 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

2.1. Computational geometry and boundary conditions

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 [64]. 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 Fig. 2(a). The detailed boundary conditions are shown in Table 2.

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 m2, was located in the middle of the room and facing the wall with air inlet and outlet. 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 [67]. 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. [64], 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 Fig. 3. During normal breathing, the opening area of mouth was about 120 ± 52 mm2 [65], but exceeded 400 ± 95 mm2 during coughing [66]. Hence, the mouth opening area was defined to be 132 mm2 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 [65]. The exhaled air and ambient air were considered as incompressible ideal gas to simulate buoyancy effect [68]. The tracer gas, carbon dioxide (CO_2) widely representing the exhaled pollutants [69], was released from the mouth with a fraction of 4.5%.

The lace of face mask was omitted in the simulations. In order tobe 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 [11,32], namely, 0.5–2.3 mm, depending on the type of face mask [17,31]. It was reported that the gap size between the face mask and face was around 4–14 mm [32], 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 [15]. Overall, the geometrical model of face mask developed in the present study is close to the reality.

2.2. Solver settings

The species transport model was used to simulate the exhaled pollutant dispersion. The discrete ordinates (DO) radiation model was applied to simulate the radiation heat transfer. The “PRESTO” scheme was used to discretize the pressure equation as it considers the pressure gradient near the boundary. Pressure-implicit with splitting of operators (PISO) algorithm was used to couple velocity field and pressure field of transient flow. The enhanced wall treatment was adopted for the wall boundary condition. The second-order upwind discrete scheme was used for other convection and diffusion terms. Convergence was achieved when the residuals reached 10□ 6 for the energy and 10□ 5 for the rest of the parameters. The CFD simulations were performed with a commercial solver, namely, ANSYS Fluent 2020R1.

2.3. Grid generation

A hybrid grid composed of polyhedron and hexahedron was adopted to fill the space. The grid of the breathing zone was locally refined, with a maximum size of 5.0 mm. The maximum y + at the human body surface was less than 2.7, with above 99% of them less than 1.0. The maximum cell size on the face mask determines whether it is fine enough to capture the detailed flow characteristics. The influence of the maximum cell size ranging between 0.8 and 8.0 mm at face mask on results was studied. Most of the exhaled air was developed as a wall-attached flow near the inner surface of face mask after hitting the face mask, meaning a high requirement for the grid refinement at the boundary layer. Hence, the sensitivity of the height of the first layer cell ranging between 0.05 and 0.50 mm at the boundary layer of face mask was examined. Within the boundary layer, the number of cell layers was set to 10.0, and the growth rate was 1.15. The grid convergence study was performed based on RANS model, and the results were verified with LES simulations. Area-averaged air speed and pollution concentration on the face mask surface (see Fig. 4(a)) were extracted and compared.

2.4. Time step size

Due to the unsteady characteristics of expiratory activities, such as breathing and coughing, both the cross-infection of infectious diseases and human inhalation exposure are transient events. Accurate simulation of the expiratory activities of individuals wearing face masks is, therefore, important. The sensitivity of the time step size ranging between 0.05 and 0.005 s for breathing and 0.05–0.0005 s for coughing was investigated. The area-averaged air speed on the face mask surface and the pollution concentration at a line with 2.0 cm away from the mouth (see Fig. 4(b)) were extracted and compared.

2.5. Turbulence model

The turbulence modeling method includes mainly two categories: the Reynolds-averaged Navier-Stokes (RANS) method and large-eddy simulation (LES) method. The Reynolds stresses (□ $\rho u'_i u'_j$) in the RANS methods was modeled by the Boussinesq hypothesis, as shown in Equation (1), yielding the turbulence models, such as S-A model (one-equation model), k-ε models (two-equation model), k-ω model (two-equation model), and transition k-kl–ω model (three-equation model). The subgrid-scale stress (τ_{ij}) in LES was also modeled by the Boussinesq hypothesis, as shown in Equation (2), yielding the subgrid-scale models (SSM) of turbulence, such as wall-adapting local eddy-viscosity (WALE) model.

In the one-equation turbulence model (S-A model), the turbulent kinematic viscosity ($\tilde{v}$) was used to compute the turbulent viscosity (μ_t). Four two-equation turbulence models were considered in the present study. As for the standard k-ε model, the turbulence kinetic energy (k) and its dissipation rate (ε) were used to compute the turbulent viscosity (μ_t). The realizable k-ε model used a modified transport equation derived from an exact equation for the transport of the mean-square vorticity fluctuation for the dissipation rate (ε). It sensitized variable (C_μ) to the mean flow and the turbulence to ensure that the model satisfies mathematical constraints on the Reynolds stresses (positivity of normal stresses and Schwarz inequality for shear stresses), consistent with the physics of turbulent flow. The renormalization group (RNG) k-ε model had an additional term (R_ε) in the ε equation than the standard model, improving the accuracy for the rapidly strained. In the shear stress transport (SST) k–ω model, the turbulence kinetic energy (k) and specific dissipation rate (ω) were used to compute the turbulent viscosity (μ_t). The SST k–ω model used a limiter to the formulation of the eddy-viscosity (μ_t) in order to account for the transport of the turbulent shear stress. In the three-equation turbulence model, the transition k-kl- ω model was used here. In this model, turbulent kinetic energy (k_T), laminar kinetic energy (k_L), and the inverse turbulent time scale (ω) were used to compute the total eddy viscosity (v_{ToT}) and the total turbulent kinetic energy (k_{ToT}). In the LES model, the

WALE model [70] was adapted. This model used spatial operator to return the correct wall asymptotic behavior for wall bounded flows, and can correct thetreatment of laminar zones.

$$-\rho u'iu'j = \mu t(\partial ui\ \partial xj + \partial uj\ \partial xi) - 2/3(\rho k + \mu t \partial uk / \partial xk)\delta ij \qquad (1)$$

$$\tau ij = -\ 2\mu t(Sij - Sij\delta ij/3) + \tau kk\delta ij/3 \qquad (2)$$

2.6. Porous media model of the face mask

The porous media model was used to simulate the airflow through face mask. This model can be used for CFD simulations of various problems related to pressure drop/loss without modeling the microscopic flow details [71]. With regard to the fluid flows through the porous media model, the source term in the momentum equation, including the viscous loss term and the inertia loss term, can be calculated as follows [72]:

$$S\mathrm{i} = -\ (\mu v\mathrm{i}/\alpha + C2\ \rho|v|v\mathrm{i}/2) \qquad (3)$$

where: α is the permeability coefficient; $1/\alpha$ is the viscous resistance coefficient; $C2$ is the inertial resistance coefficient; μ is the hydrodynamic viscosity coefficient, Pa•s; ρ is the density of the fluid, kg/m3; and v is the air speed, m/s.

The pressure drop through the porous media model can be calculated as follows:

$$\Delta P = -S\mathrm{i}\Delta n \qquad (4)$$

where: Δn is the thickness of porous media, m.

The pressure drop through face mask can also be evaluated, by the second-order polynomials, as follows:

$$\Delta P = Av^2 + Bv \qquad (5)$$

where: ΔP is the pressure drop, Pa; v is the air speed, m/s; and A and B are fitting polynomial coefficients, which can be obtained by experimental test (see Section 3.1).

The viscous resistance coefficient ($1/\alpha$) and inertia resistance coefficient ($C2$) of porous media model can be determined by solving equations (3)–(5).

2.7. Experiments for model validation

In order to verify respiratory airflow and dispersion through face mask, we measured the air speed and exhaled pollutant concentration in the breathing zone through subject experiments in an empty environmental chamber with a dimension of 5.0 m-length × 7.2 m-width × 3.0 m-height, as shown in Fig. 5(a). The subject with 1.72 m-height and 63.0 Kg-weight wearing a face mask sat on a chair, who breathed/ coughed normally via mouth during the experiments. For the breathing case, the subject maintained a normal breathing frequency (at 10–14 times/min) for 2.0 min. For the coughing case, the subject held the breath after coughing and then moved his head towards the back and sides gently and quickly to avoid the effect on coughing airflow. After the air speed and concentration decayed and stabilized, we repeated the experiment for 5 times. The wearing of face masks conformed to ordinary individual wearing habits. The commonly used surgical masks available in the market were used, which all met the relevant national standards.

In order to measure accurately the small air speed (<0.3 m/s) of the airflow through face mask, the background air speed was intentionally controlled to be a negligible level. Therefore, the mechanical ventilation was not in operation, while doors and windows were closed. In order to eliminate the influence of background concentration, a CO2 concentration monitor was arranged at a 0.2 m height from the ground in the chamber corner to record the background concentration. Considering the measuring duration was quite short (namely, in a time scale of 2.0 min) and the relatively large indoor space (namely, 108 m3), the elevation of background CO2 concentration during the experiments due to the single human subject's exhalations can be reasonably ignored. The details of the measurement instruments are shown in Table 3.

Before the experiments, all instruments were calibrated. In order to reduce the error caused by the instruments' obstruction to the airflow, the air speed and the concentration were tested separately. Fig. 5(b) and (c) shows the location of measuring points for air speed and concentration.

In addition to the experiments described above, some experimental results reported by others have also been used to further verify the simulation results. The selected experiments included the measurements of: (1) the airflow in front of face mask when the human subject was coughing (Deng and Chen [17]). In their experiments, the "patient" coughed five times in a chamber with displacement ventilation system; (2) the air leakage through face mask in the breathing zone when a thermal manikin was breathing (Shah et al. [73]). In their experiments, the exhaled air leakage was visualized through particle flow visualization and velocimetry techniques; (3) the air leakage through face mask in the breathing zone when a thermal manikin was coughing (Verma et al. [74]) and when the human subject was coughing (Koroteeva and Shagiyanova [75]). In their experiments, the exhaled air leakage was visualized through fog/smoke visualization and infrared-based human subjects over time (Gupta et al. [66]). In their experiments, a spirometer based on Fleish type pneumotachograph was used with a frequency of 330.0 Hz; (5) the cough airflow rate at 1.0 m away from the mouth of 58.0 human subjects (Dudalski et al. [76]). In their experiments, particle image velocimetry (PIV) and hot-wire anemometry (HWA) measurements were conducted.

3. Results and analysis

3.1. Boundary conditions of face mask In order to obtain the boundary conditions of face masks required by the porous media model, a small-scale literature [77,78] review on the mathematical relationship between air speed and pressure drop across a face mask was performed. As seen from Fig. 6, the area-averaged air speed through the face masks was up to

1.0 m/s in these studies. However, it has been suggested that the area-averaged air speed through the face masks during tests should be within 0.033–0.272 m/s [79]. In addition, it can be seen from Fig. 6 that, there were no sufficient test conditions at low air speed range (<0.3 m/s) in the previous studies [77, 78]. In this regard, additional experimental tests on surgical mask at low air speed range were performed in the present study and the results were also plotted on Fig. 6. Based on the mathematical relationship between air speed and pressure drop, the viscous resistance coefficient (1/α) and the inertial resistance coefficient (C2) were determined as 3.79 × 109 and 1.69 × 106, respectively. These experimentally determined coefficients were used as boundary conditions in the CFD simulations.

3.2. Influence of grid generation of face mask

Fig. 7 presents the grid distribution on the face mask and the influence of the maximum cell size at the face mask on the area-averaged concentrations on the surface of face mask. The relative deviation between the concentrations given by using the maximum cell size of 1.0 mm and 5.0 mm was 7.3%. However, it was only 3.8% between those given by using the maximum cell size of 0.8 mm and 1.0 mm. The concentration distribution on the face mask surface with the maximum cell size of 0.8 mm was also close to that of 1.0 mm, as shown in Fig. 7. In addition, the relative deviation between the air speeds given by using the maximum cell size of 0.8 mm and 1.0 mm was only □ 1.4%. Overall, these comparisons suggest that the cell size at face mask should not be larger than 1.0 mm.

Fig. 8 presents the influence of the first layer cell height at the boundary layer of the face mask on the area-averaged concentrations on the face mask surface. The cell height has only a slight influence on the concentration when the height was larger than 0.05 mm. However, it affected obviously the air speed. The relative deviation between the air speeds given by using the grids with the first layer cell height of 0.1 mm and 0.5 mm was up to 41.8%, which was much larger than that of 0.05 mm and 0.1 mm. In addition, the air speed in front of face given by the grid with the first layer cell height of 0.05 mm was very similar to that of 0.1 mm, as shown in Fig. 8(b). Overall, these results suggest that the first layer cell height at the boundary layer of the face mask should not be higher than 0.1 mm. *3.3. Determination of time step size 3.3.1. Breathing* Fig. 9 presents the influence of time step size on the area-averaged air speed on the face mask surface and the concentration in front of the face under the respiratory activity of breathing. Fig. 9(a) shows that the relative deviation between the air speeds given with the time step sizes of 0.01 s and 0.05 s was approximately 20%. However, that between the air speeds given with the time step sizes of 0.005 s and 0.01 s was only 4.0%. In addition, the results on the concentration in front of face also shows that only a slight difference existed between the time step sizes of 0.01 s and 0.005 s (as shown in Fig. 9 (b)). In general, the time step size defined for simulating the breathing activity should not be more than 0.01 s.

3.3. Determination of time step size

3.3.1. Breathing

Fig. 9 presents the influence of time step size on the area-averaged air speed on the face mask surface and the concentration in front of the face under the respiratory activity of breathing. Fig. 9(a) shows that the relative deviation between the air speeds given with the time step sizes of 0.01 s and 0.05 s was approximately 20%. However, that between the air speeds given with the time step sizes of 0.005 s and 0.01 s was only 4.0%. In addition, the results on the concentration in front of face also shows that only a slight difference existed between the time step sizes of 0.01 s and 0.005 s (as shown in Fig. 9 (b)). In general, the time step size defined for simulating the breathing activity should not be more than 0.01 s.

3.3.2. Coughing

Fig. 10 presents the influence of time step size on the area-averaged air speed on the face mask surface and the concentration in front of the face under the respiratory activity of coughing. It is found that the time step size of 0.01 s was not appropriate for coughing case, although it was fine enough to capture the flow characteristics of exhaled air for breathing case. This is strongly ascribed to that coughing has a shorter duration and a higher peak speed than breathing. The time step size of 0.001s was acceptable, with a less than 20% relative deviation between the air speeds given with the time step sizes of 0.0005 s and 0.001 s. In addition, the results on the concentration in front of face also show that only a less than 6% relative deviation near the mouth existed between the time step sizes of 0.0005 and 0.001 (as shown in Fig. 10(b)). In general, the time step size defined for simulating the coughing activity should be not more than 0.001 s.

3.4. Influence of turbulence model when breathing

3.4.1. Influence of turbulence model on velocity prediction

In order to verify the accuracy of the simulation result, the air speed passing through face masks was measured based on human subject experiments (see Section 2.7). As a whole, the simulation results calculated by different models agreed well with the experimental data, as shown in Fig. 11(a), and the maximum deviation of air speed was less than 0.05 m/s. LES model performed the best among the models examined in the present study, especially for the air speed near the face mask (L < 5 cm), where the relative deviation was only around 10%. In addition, the velocity distribution in breathing zone calculated by LES model was consistent most with the experimental results by Shah et al. [73], as shown in Fig. 12. These results indicate that the LES model is overall themodel was thus selected as the benchmark to evaluate other models.

The air speeds inside the face mask predicted by different turbulence models were compared, as shown in Fig. 11(b). Compared with LES model, the SST k-ω model performed best among the RANS models, with a 5.1% relative deviation. This finding was also applicable to the prediction of air speed near the outside of face masks, as shown in Fig. 11 (c), especially in the inspiratory phases, with less than 20% relative deviation. Fig. 11(d) shows the predicted air speed on the top of gap near nose, indicating the capability of turbulence models to capture the flow characteristics of air leakage at face mask edges. The SST k-ω model and transition k-kl-ω model obviously performed better than the S-A model and the k-ε models. These results suggest that, in addition to the LES model, the SST k-ω model can be selected to predict the airflows in and around the face masks.

3.4.2. Influence of turbulence model on concentration prediction

Fig. 13(a) shows the comparison of concentrations at locations with different distances in front of mouth, which were given by the simulations and experimental measurements. For different locations, the prediction accuracy of models was considerably different. Such a difference near the face mask ($L < 5$ cm) was evidently greater than that at locations with farther distances ($L > 10$ cm). The LES model performed the best in all models, with the closest results to the experimental data. In addition, the concentration distribution in the breathing zone predicted by the LES model was consistent most with the experimental results by Shah et al. [73], as shown in Fig. 14. The concentrations predicted by the LES model were, therefore, again selected as the benchmark to evaluate other models.

The concentrations inside the face mask predicted by different turbulence models were shown in Fig. 13(b). It can be seen that, in the inspiratory phases, the k-ε models provided the closest concentration prediction with the LES model, while the SST k-ω model had slight overestimation. Considering the best prediction accuracy of SST k-ω in speed (as presented in

Section 3.4.1), a RANS turbulence model could have inconsistent prediction accuracy in airflow and dispersion. However, different from the observations in the inspiratory phases, the prediction by the SST k-ω model agreed the best with the LES model in the expiratory phases, with only 1.5% relative deviation. In addition, Fig. 13(c) and(d) show that the SST k-ω model predicted most accurately the permeation and leakage of exhaled pollutant concentration. Overall, in view of the low computational cost and high computational robustness of RANS models, the SST k-ω model is an alternative selection for engineering applications.

3.5. Influence of turbulence model when coughing

3.5.1. Influence of turbulence model on velocity prediction

Fig. 15(a) shows the comparison of air speeds at locations with different distances in front of mouth, which were given by the simulations and experimental measurements. In general, the simulation results calculated by different models agreed well with the present experimental data and had the same trend with the results by Deng and Chen [17], especially in areas near the face mask (L < 5 cm). The air speeds obtained in the present experiment were slightly lower than those by Deng and Chen [17]. The main reason may be that different background air speeds and wearing tightness of face mask existed in the two studies. The LES model performed the best in the air speed prediction in front of mouth. Moreover, the velocity distribution in breathing zone calculated by LES model was also generally consistent with the experimental results by Verma et al. [74], as shown in Fig. 16. Slight difference in the leakage at the bottom of the face mask appears, due to the different gap sizes existed in the experiment and the simulation. Again, the results predicted by the LES model was selected as the benchmark to evaluate other models.

The air speeds inside the face mask predicted by different turbulence models were compared, as shown in Fig. 15(b). The simulation results calculated by different models were mostly in between the experimental data (at the mouth) by Gupta et al. [66] and those (at 1.0 m away from the mouth) by Dudalski et al. [76]. This indicates that all turbulence models can roughly capture the momentum characteristics of coughing. For the air speed outside the face mask, all models (except the SST k-ω model) performed poorly, as shown in Fig. 15(c). However, for the air speed inside the face mask and on the top of gap near nose, all models performed well, as shown in Fig. 15(b) and (d). Among those models, the SST k-ω model again shown the best prediction accuracy, with around 13% relative deviation for the air speed near the outside of the face mask. Overall, among RANS models, the SST k-ω model is a good choice for predicting coughing airflow.

3.5.2. Influence of turbulence model on concentration prediction

Fig. 17(a) shows the comparison of concentrations at locations withconcentration distribution in breathing zone predicted by the LES model was also supported by the experimental results by Koroteeva and Shagiyanova [75], as shown in Fig. 18. This implies that the LES model has a good prediction accuracy. The concentrations predicted by the LES model were, therefore, again selected as the benchmark to evaluate other models.

The concentrations inside the face mask predicted by different turbulence models were shown in Fig. 17(b). Compared with LES model, the SST k-ω model, the k-ε models, and the transition k-kl-ω model performed well in the early stage of coughing ($t < 0.3$ s). However, those models cannot well capture the characteristics of concentration decay in the late stage of coughing ($t > 0.3$ s). This observation has been confirmed again in the predicted concentrations outside the face masks, as shown in Fig. 17(c). For the concentration leakage at face mask edges, all models performed well, especially the SST k-ω model, as shown in Fig. 17(d). In general, RANS models can predict the concentration decay well only in the early period of coughing.

4. Discussion

4.1. Geometric modeling, gird division and boundary conditions of face mask

The commonly used face masks in the market are made of soft materials, including non-woven fabric (such as meltblown polypropylene), cotton, cloth, etc. [3] The face masks are therefore easy to be deformed in real life, depending on the wearer's pressing level for making the face mask fit the face. At present, the geometric modeling methods mostly simplify the geometry of the face masks to have smooth hemispherical surface [11,35], smooth face-shaped surface [37], and smooth face-shaped surface with folds [31,32]. In the present study, a smooth face-shaped surface that fits the face more realistically was used. However, the shape deformation of face masks due to exhaled air during use was not considered in past simulations. This is worthy of further exploration.

In addition to geometric modeling, gird generation is also important. The gird types used in the existing studies on face masks include tetrahedron [31,44], polyhedron [24], etc. In the present study, the mixed gird of polyhedron and hexahedron was used to fill the face mask space for its good adaptability in irregular geometry. In addition, the gird independence in the division process was evaluated in past studies mostly based on the total gird number of the whole room, but the specific cell size and distribution on face mask as well as their independence test were rarely given. The present study reported that the cell size at face mask and the height of the first layer cell near face mask should not be larger than 1.0 mm and 0.1 mm, respectively.

Modeling method of flow characteristics through face masks with a microporous structure, can be divided into two methods: direct method [30] and indirect method [24,28,44]. The direct method is to establish a real microporous structure of the face mask. However, due to a large number of complex holes to be built in the direct method model, the indirect method based on porous media model was adopted in most simulation studies. In the present study, based on experimental tests, the boundary conditions of the face mask used in the porous media model were determined. Summing up, the geometric modeling, gird division, and boundary conditions are important computational parameters that influence largely the accuracy of CFD prediction of problems related to face masks. The new insights obtained and developed in the present study would provide method and basis for the determination of these parameters.

4.2. Validation experiment of the face mask simulation

Model validation is particularly important for numerical simulation. However, most previous studies on the simulation of face masks lack systematical experimental validation. Moreover, the use of only indoor airflow data for model validation is insufficient to justify the simulation of airflow and dispersion around face masks. In the present study, the model validation is performed in the following three main aspects: the decay of air speed with distance after the exhaled airflow penetrating through the face mask, the decay of concentration with distance afterthe exhaled airflow penetrating through the face mask, and the visualization of air leakage around the face mask. They provide a comprehensive validation for the accurate simulation of face masks. However, it has to be noted that there is still a lack of quantitative experimental data on air leakage at the face mask edges for model validation.

To have a complete experimental validation of CFD simulation of face masks, three aspects should be included: air leakage at the face mask edges, air penetration through face mask surface, and the microenvironment under face mask. First, it is difficult to measure the air leakage at the face mask edges by directly arranging instruments. The commonly appropriate methods include infrared-based visualization [75], smoke visualization [16,74], and PIV technology. Second, for the measurement of air penetration through face mask surface, intrusive instrument measurement (e.g., hot-wire anemometry) [17] and PIV technology [80] are useful and appropriate methods. Finally, for the microenvironment under face mask, the intrusive measurements through external measuring tube from the gaps around the face mask edges based on human subject and through internal measuring tube based on thermal manikin [81] are the most appropriate methods. The subject experiments can best reflect the real expiratory activities and the fitness between the face mask and the face. However, its repeatability is weak, and it is difficult for a subject to maintain a posture for an extended period. In contrast, the manikin experiment is easy to operate and control, but has some deviations from the reality. It is worth to mention that the model validation through similarity experiment has been applied to respiratory jet. Liu et al. [82] had a good validation case for respiratory jet based on a water channel experiment. In general, the basic experimental database as well as reliable methods for model validation of thermos-fluid performance of face masks should be established.

4.3. Adaptability of turbulence model

The results obtained in the present study show that the LES model is most accurate for the simulations related to breathing and coughing when wearing a face mask. This is attributed to the fact that this model computes the large energy-carrying eddies whereas models only the small subgrid scales of motion. The small scales tending to be more isotropic and homogeneous than the large ones, and thus more amenable to universal modeling [83]. However, the main shortcoming of LES model lies in the high resolution requirements for wall boundary layers [83]. It brings large computing costs and computing resources, limiting its engineering applications. Compared with LES model, the SST k-ω model has the overall best accuracy among the RANS models in the prediction of airflow and dispersion through face masks.

The use of face mask results in considerable differences in the flow characteristics at different areas in the breathing zone when compared to those without face mask. The existing turbulence models cannot always predict accurately the different expiratory activities in different areas. For complex flow problems, researchers have proposed methods including hybrid models (e.g., Scale-Adaptive Simulation (SAS) [84], Detached Eddy Simulation (DES) [85]), and embedded models (e.g., embedded Large Eddy Simulation (ELES) mode [86]). As for hybrid models, the switching parameter can of course be adjusted by anempirical coefficient, but the desired criterion is difficult to know in advance for unknown complex flows [87]. As one of the classical embedded models, ELES has a clear distinction from the RANS and LES regions even during the grid generation phase. In view of the nonuniform distribution of airflow and dispersion in terms of spatial and time scales, namely, near-wall and main airflows in space as well as high-speed and low-speed airflows over time, developing advanced hybrid or embedded models for respiratory airflow and dispersion through face mask, even other PPE, is the key to achieve high-precision and low-cost simulations.

4.4. Limitations

Several limitations have to be clarified. First, the tracer gas is used in the present study to represent the exhaled gaseous and fine particle pollutants, while large droplets were not considered. Second, the turbulence models compared in the present study are those commonly used in past studies on PPE simulation, but some other models, such as different sub-category LES models, are not fully examined. Third, several different sets of available experimental data in the literature are used to validate the present CFD simulations, but there are some differences between the conditions of experiments and simulations. Finally, various types of face masks are also not fully explored.

5. 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 × 109 and 1.69 × 106, 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.

CRediT authorship contribution statement

Zhongjian Jia: Writing – original draft, Visualization, Validation, Software, Resources, Methodology, Investigation, Formal analysis, Data curation. **Zhengtao Ai:** Writing – review & editing, Writing – original draft, Supervision, Resources, Project administration, Methodology, Funding acquisition, Conceptualization. **Xiaohua Yang:** Writing – review & editing, Methodology. **Cheuk Ming Mak:** Writing – review & editing, Methodology. **Hai Ming Wong:** Writing – review & editing, Methodology. **Declaration of competing interest** The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper. **Data availability** Data will be made available on request.

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