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Modelling of evaporation of cough droplets in inhomogeneous humidity fields using the multi-component Eulerian-Lagrangian approach

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Abstract

This study employed a multi-component Eulerian-Lagrangian approach to model the evaporation and dispersion of cough droplets in quiescent air. The approach is featured with a continuity equation being explicitly solved for water vapor, which allows comprehensively considering the effects of inhomogeneous humidity field on droplets evaporation and movement. The computational fluid dynamics (CFD) computations based on the approach achieved a satisfactory agreement with the theoretical models reported in the literature. The results demonstrated that the evaporation-generated vapor and super-saturated wet air exhaled from the respiratory tracks forms a "vapor plume" in front of the respiratory track opening, which, despite the short life time, significantly impedes the evaporation of the droplets captured in it. The study also revealed that due to the droplet size reduction induced by evaporation, both the number density of airborne droplets and mass concentration of inhaling pathogens remarkably increased, which can result in a higher risk of infection. Parametric studies were finally conducted to evaluate the factors affecting droplet evaporation.

Summary: The study demonstrated the importance of considering inhomogeneous humidity field when modeling the evaporation and dispersion of cough droplets. The multi-component Eulerian-Lagrangian model presented in this study provides a comprehensive approach to address different influential factors in a wide parametric range, which will enhance the assessment of the health risks associated with droplet exposure.

Keywords: Cough droplets, Evaporation, Dispersion, Time-dependent droplet size, Inhomogeneous humidity field, Multi-component Eulerian-Lagrangian model

1. Introduction

Transmissible respiratory diseases such as influenza, tuberculosis (TB) and severe acute respiratory syndromes (SARS) are serious threats to the public health due to their high morbidity and mortality. The survey by Palache et al. [1] estimated that the influenza A virus (IAV) alone causes around 5 million infection cases globally every year, resulting in 250,000 to 500,000 annual deaths. Since the airborne routes play a key role in spreading respiratory pathogens from person to person, an enhanced understanding of pathogen transmission via aerosolized sputum and saliva droplets is vital to the public health measures aiming at reducing infection risks.

Droplets generated from human respiratory activities are distributed in a wide size range. According to the experimental measurements by Gralton et al. [2], the droplets generated from human coughing, sneezing and talking are mostly between 1 nm and 500 μm. The diameter is a critical parameter determining the fate of the droplets because droplets larger than 100 μm would quickly settle while those smaller than 100 μm could become airborne and have the chance to be inhaled [3]. For airborne droplets, their movement could be dominated by the inertial and gravitational effects or the airflow, depending on the droplet size and air velocity [4]. In addition, studies on particle deposition in human airways [5] have proven that particles larger than 10 μm tend to impact onto the surface of upper airways while those smaller than 10 μm are more likely to penetrate deeper into the lower airways and pulmonary region. Some investigators [2,3] hence recommended 10 μm as a cut-off diameter to delineate upper and lower respiratory tract infections. Apparently, appropriate characterization of droplet size is of great importance to the assessment of health risks based on droplet trajectories [6], and to the analyses of individual health hazards associated with particulate exposure.

Respiratory droplets are composed of water and a small amount of non-volatile compounds including sodium chloride, carbohydrate, lipids, protein and microorganisms [7,8]. After being expelled, water in the droplets would gradually evaporate and finally leave behind the non-volatile components to form solid droplet nuclei. The equilibrium diameter of a completely desiccated droplet nucleus $d_{4d}$ is correlated to its initial diameter $d_{4i}$ by Ref. [9].
\[ d_{e,c} = \left( \frac{C_{sw}}{\rho_{sw}} \right)^{1/3} d_{d,0} \]  

A common estimation of the droplet density and initial concentration of non-volatile compounds is \( \rho_{sw} = 1000 \text{ kg/m}^3 \) and \( C_{sw} = 1.8\% \) [8], which results in an equilibrium diameter of \( d_{e,c} = 0.262d_{d,0} \). This means that as water evaporates, some free-falling large droplets could become airborne [10], leading to an elevated number density of inhalable droplets in the breathing zone and an increased probability of infection [11,12].

The evaporation of droplets is driven by the equilibrium vapor pressure on the droplet surface relative to the partial pressure of water vapor in the ambient air [9]. This process is strongly controlled by the droplets specific area and ambient conditions including the air temperature, humidity and turbulence. The calculation by Wei and Li [13] revealed that a droplet with an initial diameter of 10 \( \mu \text{m} \) needed only 0.07 s to reach its equilibrium diameter in dry air (0% relative humidity, RH) while a 100-\( \mu \text{m} \) droplet required over 100 s to complete the same process in 90% RH air. Given that the size of a droplet significantly determines its movement and fate, plus the fact that the viability of viruses within the droplet is affected by the moisture content and temperature [3,14], an effective modelling of the time-dependent droplet size is crucial to the assessment of health risks associated with droplets exposure, for both the public and individual interests.

Despite the importance of droplets in transmitting respiratory disease has long been recognized, the theoretical models and experimental data on respiratory droplets are still very scarce, particularly in terms of the evaporation and dispersion. The classic Wells evaporation-falling curve (1934) [15] was widely used to estimate the droplet size as a function of time. However, Xie et al. [16] suspected that the curve was plotted based on experimental results through extrapolation using various inappropriate assumptions. In recent years, a couple of mathematic models [7,9,13,16] were developed in which the effects of respiratory jets, air turbulence, droplet salinity and ambient humidity were partially considered. However, most of these models simply ignored the inhomogeneous humidity field induced by the evaporating droplets and the supersaturated water vapor exhaled from the respiratory tracts. Although some theoretical models, such as that of Chao and Wan [17], employed a transportable scalar to model the concentration diffusion of water vapor in air, the effects of inhomogeneous water vapor concentration on droplet evaporation were not fully addressed. In fact, the inhomogeneous vapor concentration, particularly in the immediate vicinity of the droplets, may have a strong effect on the droplet trajectories through changing the time-size relationship. In addition, the transport characteristics of water vapor in the air may be subjected to many factors including the air pressure and temperature, as well as the vapor concentration itself [18]. A transportable scalar may be inappropriate to model the transport behaviours. This is particularly true when the local vapor concentration is high. In order that droplet evaporation and transport could be modelled in a systematic way, the diffusion of water vapor in the air needs to be modelled mechanistically.

In this study, the multi-component Eulerian-Lagrangian approach was employed to realize a mechanistic modelling. Compared with the existing models reported in the literature, the approach is unique as a continuity equation was explicitly solved for the water vapor. Although droplets can be expelled through various respiratory activities such as breathing, coughing, sneezing and talking, only cough was considered in this study as it is a common symptom of most respiratory infections and the major source of pathogen-carrying droplets in indoor air [19]. Other important factors including the exhaled humidity, expelled droplets amount, ambient humidity and temperature were also discussed.

2. The multi-component Eulerian-Lagrangian model

2.1. Governing equations

In the multi-component Eulerian model, the wet air is treated as an ideal mixture composed of dry air and water vapor. All the thermodynamic properties of the mixture are calculated by

\[ \varphi_m = f_m \varphi_a + f_a \varphi_v \]  

where, the subscripts \( m, a \) and \( v \) denote the air-vapor mixture, dry air and water vapor, respectively. \( \varphi \) represents a property parameter (\( \varphi = \rho, \mu, \lambda, \varepsilon, \gamma \) etc) and \( f \) is the mass fraction (\( f_a + f_v = 1 \)).

To capture the transport characteristics of water vapor through the air, continuity equations for the dry air and water vapor are solved separately

\[ \frac{\partial}{\partial t} (\rho_m \mathbf{U}_m) + \nabla \cdot (\rho_m \mathbf{U}_m \mathbf{U}_m) = 0 \]  

where, \( \mathbf{U}_m \) is the mass-averaged mixture velocity. \( S_m \) is the mass source of water vapor due to droplets evaporation. \( D_h \) is the kinematic diffusivity of water vapor in the air.

Since air and water vapor are mixed at the molecular level, it’s safe to assume they share the same local velocity, pressure and temperature, which allows solving only one momentum and energy equation for the mixture

\[ \frac{\partial}{\partial t} (\rho_m \mathbf{U}_m) + \nabla \cdot (\rho_m \mathbf{U}_m \mathbf{U}_m - \rho_m \mathbf{U}_m + (\nabla \mathbf{U}_m) \nabla) = S_{\text{Bouy}} + S_{\text{int}} - \nabla p \]  

where, \( S_{\text{Bouy}} \) is the momentum source due to buoyancy, \( S_{\text{int}} \) is the interfacial forces acting on the droplet interfaces, \( \nabla p \) is the pressure gradient, \( H_m \) is the mixture enthalpy, \( T_m \) is the mixture temperature and \( Q_{\text{int}} \) is the interphase heat transfer rate across the droplet interfaces.

For a unit control volume containing \( N \) droplets, the interfacial heat transfer rate between the phases is calculated by

\[ Q_{\text{int}} = \sum_{n=1}^{N} \mathcal{W}(\mathcal{N}_d \mathcal{W}_d \mathcal{W}_d - \mathcal{N}_d \mathcal{W}) \]  

where, the subscripts \( d \) are the droplet diameter, \( \mathcal{W}_d \) is the droplet temperature and \( \mathcal{W}_d \) is the interfacial heat transfer coefficient estimated according to Ranz and Marshall [20].

\[ N_d = \frac{h_m d_d}{\lambda_m} = 2 + 0.6 \text{Re}_d^{0.5} \text{Pr}_m^{1/3} \]  

where, \( \text{Re}_d \) and \( \text{Pr}_m \) are the droplet Reynolds number and the mixture Prandtl number, respectively.

The movement of droplets is tracked using the Lagrangian approach. For micron-sized droplets with a density much higher than that of the carrying fluid, the interfacial forces depending on the density ratio are negligibly small [21]. Therefore, only the buoyancy force \( F_{\text{Bouy}} \) and drag force \( F_D \) are considered and the equation of droplet motion is defined by

\[ m_d \frac{d \mathbf{U}_d}{dt} = F_{\text{Bouy}} + F_D \]  

\[ F_{\text{Bouy}} = \frac{\rho_d d_d^2}{6} (\rho_d - \rho_m) g \]  

\[ F_D = \frac{C_{\text{D}} d_d^2}{2} \frac{\rho_d g}{4} \mathcal{W}_d - \mathcal{U}_d \mathcal{W} \mathcal{W}_d (\mathcal{W}_d - \mathcal{U}_d) \]  

where, \( \mathcal{U}_d \) is the droplet velocity.
The turbulent dispersion of droplets was modelled in this study by adding a turbulence fluctuating component, which is correlated to the turbulence kinetic energy $k$ and a normally distributed random number $\Phi$, onto the mixture velocity.

$$\tilde{U}_{in} = \overline{U}_{in} + \Phi \sqrt{\frac{2k}{3}}$$  \hspace{1cm} (12)

### 2.2. Droplet evaporation model

The expelled saliva/phlegm droplets are assumed to be composed of 98.2% water and 1.8% non-volatile solid compounds, according to Nicas et al. [8]. The evaporation of water is controlled by the equilibrium vapor pressure at the droplet surface relative to the ambient pressure. When the effects of non-volatile compounds were ignored, the equilibrium vapor pressure at the droplet surfaces is calculated using the Antoine equation

$$p_{ev} = p_{scale} \exp \left( \frac{A - B}{T_e} + C \right)$$  \hspace{1cm} (13)

where, $p_{scale}$ is the pressure scale. $A$, $B$ and $C$ are the Antoine constants. When $p_{scale} = 1.0$ bar, the constants take values of $A = 12.439$, $B = 4233.7$ and $C = -31.737$ according to Bridgeman and Aldrich [22]. For droplets suspended in common indoor air, their evaporation is subject to the diffusion mechanism and the mass transfer rate is calculated by

$$\frac{d m_d}{dt} = -\frac{dS_v}{dt} = -\pi d_d D_{dyn} Sh \frac{M_v}{M_m} \ln \frac{1-X_{v,m}}{1-X_{v,l}} - \pi d_d D_{dyn} Sh \frac{M_v}{M_m} \ln \frac{P - P_{ev}}{P - P_{fl}}$$  \hspace{1cm} (14)

where, $D_{dyn}$ is the dynamic diffusivity of water vapor in the continuum. $Sh$ is the Sherwood number [20]. $M_s$ and $M_m$ are the molecular weights of the vapor and the mixture, respectively. $X_{v,i}$ is the equilibrium mole fraction of water vapor at the droplet surface and $X_{v,m}$ is the local mole fraction of water vapor in the mixture, which can be represented by the partial pressures of water vapor at the droplet surface $p_{v,c}$ and in the mixture $p_{v,m}$, respectively.

When the temperature gradient inside a droplet is ignored, the temperature decrease of the droplet due to the latent heat of phase change is expressed by

$$m_{u,c} \overline{a} \frac{dT_d}{dt} = q_{mol} - h_{\alpha} \frac{dm_d}{dt}$$  \hspace{1cm} (15)

### 2.3. Numerical procedures

A chamber representing a cuboid space in front of a coughing person was assumed, as shown in Fig. 1. The chamber was created big enough (4 m-length × 2 m-width × 3 m-height) so that the airflow was free from the effects of the no-slip chamber walls. No ventilation was designed in order to create a quasi-quiescent environment. Droplets were injected through a nozzle which was located 2.0 m above the floor. The diameter of the nozzle was 2 cm representing a coughing human mouth opening. The other end of the chamber opposite to the nozzle was open to the atmosphere, allowing taking into account the ambient conditions such as the air temperature and humidity. Non-reflecting boundary conditions were specified at all the solid chamber walls, which acted as a sink term of droplet mass when the droplets hit the walls.

Due to the symmetric distribution of the airflow field, only half of the chamber was built as the computational domain with the central plane ($Y = 0$ m) being set as a symmetric plane (Fig. 1). The domain was then discretized using structured hexahedral grids with very fine mesh applied in the near-wall regions. Mesh independence was achieved at 500,000 mesh elements because a further increase to 600,000 mesh elements only produced a negligible change (less than 0.5%) in the predicted air velocity and vapor concentration profiles along a randomly selected line. The number of droplet trajectories was also analysed. It was found that when the trajectory number was larger than 20,000, the predicted vapor concentration field was free from the number. The model equations were discretized based on a finite-volume method and solved using the commercial CFD code CFX-17, together with the RNG $k$-$

### 3. Results and discussion

#### 3.1. Model validation

The evaporation of droplets falling freely in quiescent air was firstly simulated for model validation. During the computations, two single droplet seizes (10 and 100 μm) and very small droplet mass flow rates ($5.24 \times 10^{-11}$ kg/s for the 10-μm droplets and $5.24 \times 10^{-8}$ kg/s for the 100-μm droplets, respectively) were used in order to match the computational conditions of Wei and Li [13], who assumed single droplets were released one after another with a time interval of 0.01 s. Computations were conducted with a constant temperature of 25 °C and different air humidity (RH = 0% and 90%) conditions, respectively.

The predicted time-dependent droplet diameter (solid lines) was compared against the theoretical calculations (dot points) by Wei and Li [13] and Redrow et al. [7], as shown in Fig. 2. Satisfactory agreement was obtained between the numerical results of this study and the data reported in the literature, for the both initial droplet size and air relative humidity. The figures also reveal that the evaporation of droplets is sensitive to the both parameters considered here. Firstly, the evaporation rate is strongly affected by the droplet size. Smaller droplets evaporate much faster than larger droplets because of the enlarged specific surface area for heat and mass transfer. Secondly, the relative humidity of air plays an important role. When the relative humidity increased from 0% to 90%, the time required for the droplets to reach their equilibrium diameters tremendously increased from 0.065s to 0.45s (692% increment) for the 10-μm droplets and from 4.0s to 28.0s (700% increment) for the 100-μm droplets.

#### 3.2. Parametric study

It was noted that the above validation computations were conducted with very small droplet mass flow rates ($5.24 \times 10^{-11}$ kg/s and $5.24 \times 10^{-8}$ kg/s, respectively). With such small mass flow rates, it was safe to ignore the effects of inhomogeneous humidity field [6]. However, coughing is featured with an instantaneous pulse airflow carrying water vapor and droplets coming from the respiratory tracts. Due to the supersaturated wet air (5% water vapor) and droplets evaporation, the respiratory droplets are actually dispersed in a...
heterogeneous humidity field, particularly in the region close to the respiratory tract openings (mouth and nostrils). Apart from that, many other factors including the mass of exhaled droplets, the ambient temperature and humidity could have significant effects on the process of droplet evaporation, resulting in different time-size correlation and droplet dispersion trajectories. In this section, parametric studies were performed to evaluate the effects of each individual factor.

In order to capture the dynamic characteristics of cough and droplets evaporation, transient simulations were conducted. A pulse air jet representing a single cough was applied at the nozzle according to the experimental data of Gupta et al. [19]. The pulse air jet had a time duration of 0.5 s and a peak flow rate of 4.2 L/s at $t = 0.08$ s (Fig. 3(a)), which generated a peak air velocity of 13.4 m/s at the nozzle. Droplets were injected into the domain with the same instantaneous velocity of the pulse airflow. Given that the droplets expelled by human cough are dispersed in a wide size range, the number and mass probability density distributions of droplets between 3 and 750 μm (Fig. 3(b)), which were measured 10 mm in front of the mouth opening by Chao et al. [24],

were employed to specify the droplet injection conditions. It was noticed from Fig. 3(b) that over 80% of the droplets expelled by a human cough are smaller than 30 μm. However, these small droplets only account for around 0.1% of the expelled liquid mass.

For the purpose of comparison, a baseline computation (Case 1) was firstly conducted without considering the inhomogeneous humidity field, namely, $f_v = 0$ and Eq. (4) being not solved. Then, the evaporation-generated water vapor and exhaled water vapor (5% mass concentration [25]) was progressively added to Case 1 (Case 2 and 3). Finally, computations were also conducted to parametrically evaluate the effects of the expelled droplet mass (Case 3–5) and ambient temperature (Case 3, 6–8) and humidity (Case 3, 9 and 10). The boundary conditions of each computational case are listed in Table 1.

During the computations, very small-time steps (0.01 s) were used in the beginning in order to capture the instantaneous cough jet (0.5 s). The time steps then gradually increased up to 1.0 s. The total droplet tracking time was 30 s, which took around 30 h to run a single simulation on a workstation with 40 CPU cores (2.8G Hz Intel® Xeon®) and 128 GB RAM.

3.2.1. The effects of inhomogeneous humidity field

The effects of locally elevated water vapor concentration on the evaporation and dispersion of droplets were analysed through comparing the results yielded from Case 1, 2 and 3. The predicted transient air velocity vectors and water vapor concentration contours in a small
rectangular area (2 m-length × 1.2 m-height) next to the nozzle are shown in Fig. 4 (Case 3). The results revealed that the cough created a strong pulse air jet, which, however, quickly faded away in the quiescent air. The maximum air velocity decreased from 13.3 m/s at t = 0.08 s to 1.16 m/s at t = 8.0 s. The cough also remarkably elevated the local air humidity due to the exhaled wet air, creating an instantaneous “vapor plume” in which the vapor concentration is significantly higher than that in the bulk air. Fig. 4 shows that the vapor plume, analogous to the air jet, also quickly dissipated so that at t = 8.0 s no significant gradients of vapor concentration can be observed. However, despite its short life, the vapor plume was found to have a significant effect on the evaporation and dispersion characteristics of droplets, particularly on those of the small droplets.

Shown in Fig. 5 are the droplet trajectories predicted without and with vapor transport (Case 1 and 3), respectively. The results show that the diameter of 100 μm acted as a critical size for droplet movement as droplets smaller than 100 μm were steadily suspended in the air and dispersed by the air turbulence, while the movement of droplets larger than 100 μm was jointly controlled by the gravitational and inertial effects. As shown in Fig. 5, droplets larger than 100 μm were free falling and quickly settled onto the floor following smooth trajectories analogous to parabolic curves. The locally elevated air humidity seemed to have no noticeable effects on the trajectories of these large droplets. Thus, the diameter of 100 μm can be treated as a cut-off size to delineate airborne and free-falling droplets, which is in accordance with the recommendation of Weber and Stilianakis [3].

However, for the airborne droplets with diameter smaller than 100 μm, the inclusion of vapor transport in the computational model could result in different predictions of evaporation and dispersion. As shown in Fig. 5, when the inhomogeneous humidity field was considered, the airborne droplets were predicted to travel faster and further than predicted without water vapor transport. When the transport equation of water vapor (Eq. (4)) was included, the airborne droplets were predicted to have travelled up to 0.65 m at the end of the cough (t = 0.5 s), which was 18% larger than the maximum travelling distance (0.55 m) predicted without vapor transport. Although the airborne droplets soon lost their momentum due to the decreasing air velocity, the predicted particle travelling distance was still 14% larger at t = 8.0 s when the inhomogeneous humidity was considered. Referring to Fig. 4, it seems that the locally elevated air humidity is beneficial for maintaining the droplets’ momentum and inertia.

It was noted the “droplet plume” in Fig. 5 had a comparable size to that of the “vapor plume” in Fig. 4. This means that the airborne droplets were completely located in humid air in the following few seconds after a cough, which can certainly hinder their evaporation. Fig. 6 shows the size variation of the 12-μm droplets after expulsion. When the inhomogeneous humidity field was ignored (Case 1), the droplet median evaporation time was only 0.12 s. The evaporation rates of all the droplets were predicted to be similar, so that the time-dependent droplet sizes were distributed in a narrow area near their average value. In addition, the curves of the average and median sizes were almost overlapping with each other, meaning that the droplets were predicted to evaporate at the same speed. However, when the inhomogeneous humidity field induced by droplets evaporation was considered (Case 2), the median evaporation time was significantly prolonged (0.29 s). The time-dependent droplet sizes were predicted to be dispersed in a much wider range, suggesting different evaporating rates of the droplets despite the same initial diameter. As shown in Fig. 6(b), some droplets only needed 0.15 s to completely evaporate while some others spent as much as 6.0 s to accomplish the same process. Because of this, the average droplet size was predicted to decrease significantly slower than the median size. Finally, the inclusion of the exhaled humidity further decreased the predicted droplets evaporation rate (Fig. 6(c)), particularly the droplet median evaporation time was significantly prolonged.

The effects of inhomogeneous humidity field on the time-dependent median size and temperature of two selected groups of droplets (12-μm and 112-μm) are shown in Fig. 7. When the evaporation-induced humidity was considered, the time required for 50% of the 12-μm droplets to completely evaporate increased from 0.12 s to 0.29 s (142% increment), which further increased to 0.54 s when the exhaled vapor was added (208% additional increment). Comparatively, the time-dependent size of the 112-μm droplets was not significantly affected by the inhomogeneous humidity field, probably because the travelling speed of this group of droplets was larger than that of vapor dispersion (refer to Figs. 4 and 5), so that they were travelling outside the vapor plume and their evaporation was not affected by the locally elevated water vapor concentration.

Fig. 7 clearly demonstrates that the comprehensive consideration of the inhomogeneous humidity field is critical to an effective modelling of droplet evaporation and dispersion. Therefore, both the exhaled water vapor and evaporation-generated water vapor were included in the following computational cases.

### Table 1

| Case No. | Vapor Transport? | Ambient conditions | Exhaled humidity | Droplets amount |
|---------|------------------|--------------------|-----------------|----------------|
|         |                  | T (°C)  | RH (%) | (°v) | (mg) |
| 1       | No               | 25     | 50    | 0    | 100  |
| 2       | Yes              | 25     | 50    | 0    | 100  |
| 3       | Yes              | 25     | 50    | 5    | 100  |
| 4       | Yes              | 25     | 50    | 5    | 1000 |
| 5       | Yes              | 25     | 50    | 5    | 1000 |
| 6       | Yes              | 25     | 50    | 5    | 100  |
| 7       | Yes              | 25     | 50    | 5    | 100  |
| 8       | Yes              | 25     | 50    | 5    | 100  |
| 9       | Yes              | 25     | 50    | 5    | 100  |
| 10      | Yes              | 25     | 90    | 5    | 100  |

3.2.2. The effects of expelled liquid amount

The effects of expelled droplets amount were also investigated (Case 3–5). Although the experimental data on how much salivary or phlegmy droplets can be expelled by a single cough is still unavailable in the open literature, it is reasonable to estimate that this amount could be as high as hundreds of milligrams according to the high-speed CCD images (Fig. 8) of Bourouiba et al. [26]. Therefore, computations were conducted with three different droplet masses (10, 100 and 1000 mg) corresponding to mild, moderate and severe coughs, respectively.

Fig. 9 shows the contour maps and droplet trajectories predicted with different droplet masses. Only the trajectories of airborne droplets (smaller than 100 μm) were shown in the figure to improve the illustration clarity. The results firstly revealed that the increased droplet...
mass noticeably enlarged the size of the high-humidity area and the maximum vapor concentration in the domain. At $t = 2.0$ s when the exhaled humidity had fully dispersed, the evaporation of the droplets was still significantly elevating the local humidity. As shown in Fig. 9 (a), the maximum local mass concentration of water vapor reached 1.60% when the droplet mass was 100 mg (Case 3). If the droplet mass could increase up to 1000 mg, the maximum local vapor mass concentration could reach as high as 1.97%, which was the saturated water vapor concentration in the air at the given temperature and pressure conditions (25 °C and 101.325 kPa). The increased droplet mass also changed the droplet trajectories. As shown in Fig. 9 (b), the gravitational settlement of droplets became more significant. Particularly, when the mass flow rate of droplets increased to 1000 mg, the droplets presented a remarkably changed distribution pattern, which will certainly result in different risk assessments if the assessments were based on droplet trajectories [27].

The time-dependent sizes of the representative droplets (12-μm and 112-μm) are shown in Fig. 10. The results demonstrated that the increased droplet mass significantly prolonged the median evaporation.

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Fig. 5. Droplet trajectories predicted with and without vapor transport.
(a) Case 1 (Without vapor transport).
(b) Case 3 (With vapor transport).

Fig. 6. The predicted time-dependent diameter of the 12-μm droplets.
(a) Case 1.
(b) Case 2.
(c) Case 3.

Fig. 7. The effects of inhomogeneous humidity field on the time-dependent sizes of droplets.
time of the 12-μm droplets. The time required for 50% of the 12-μm droplets to completely evaporate was 0.42, 0.56 and 1.26 s, respectively, when the exhaled droplet mass was 10, 100 and 1000 mg. However, the 112-μm droplets seemed unaffected by the droplet mass.

### 3.2.3. Effects of the ambient conditions

Computations were also conducted with different ambient conditions. The ambient temperature and humidity ranges were 5–35°C and RH 10–90% (Case 3, 6–10), respectively. Such a wide parametric range was selected to cover the worst-scenario conditions.

The time-dependent sizes of the representative droplets predicted with different ambient temperature and humidity are shown in Figs. 11 and 12, respectively. The results demonstrated that the evaporation of droplets, particularly airborne droplets, is sensitive to the both ambient parameters. At a relative humidity of 50%, the increasing ambient temperature can observably accelerate the droplet evaporation (Fig. 11). When the ambient temperature increased from 5°C to 35°C, the median evaporation time of the 12-μm droplets decreased from 1.44 s down to 0.42 s (71% decrease). Although under all the 4 selected ambient temperatures, the 113-μm droplets did not fully evaporate as they settled quickly onto the floor, their final median size decreased to 95, 91, 77 and 70 μm, respectively, when hitting the floor (Fig. 11).
indicating significant evaporation.

The ambient humidity also has a strong effect on the rate of droplet evaporation. As shown in Fig. 12, when the ambient relative humidity decreased from 90% to 10%, not only the median evaporation time of the 12-μm droplets significantly dropped from 3.15 s down to 0.33 s, but also 50% of the 112-μm droplets were completely evaporated within 9 s and became steadily airborne. However, the 112-μm droplets only slightly evaporated in the RH 90% air, so that their median diameter was still 108 μm when hitting the floor, which was only 3.5% smaller than their initial size. According to Figs. 11 and 12, it seems that the ambient humidity plays a more important role in affecting the rate of droplet evaporation than the ambient temperature does.

3.3. Analysis of inhalable pathogen

The computational results show that due to the evaporation-induced size reduction, some large free-falling droplets (larger than 100 μm) could become airborne (smaller than 100 μm) and hence improve the number density of inhalable droplets in the domain (Fig. 13). Some of these new airborne droplets and nuclei could be entrained into the breathing zone by uprising airflows such as the human thermal plume. Due to the large mass of pathogens carried in these type of new airborne droplets/nuclei, the possibility of infection can be significantly increased. Similarly, some small airborne droplets could further shrink in size, becoming smaller than 10 μm and increasing the probability of lower respiratory tract infections [5].

Fig. 14 shows the time-dependent number fraction of airborne droplets/nuclei (smaller than 100 μm). The mass fraction of inhalable pathogen, which is defined as the pathogen carried by the airborne droplets/nuclei, is also shown in the figure. It was demonstrated that although the airborne droplets took a predominant number proportion (0.90) of the exhaled droplets, they only accounted for a very small mass fraction (2.18 × 10⁻³) of the total mass of expelled pathogen. When the ambient relative humidity was medium (Fig. 14(a), RH 50%), although the total number fraction of inhalable droplets/nuclei and total mass fraction of inhalable pathogen did not change till 10 s after the cough, the number fraction of small droplets/nuclei (smaller than 10 μm) increased from 0.60 to 0.87 while the mass fraction of the inhalable pathogens carried by them significantly increased from 4.89 × 10⁻⁷ to 1.58 × 10⁻⁴, which was an astonishing 323-fold increase. When the ambient air had a low relative humidity (RH 10%), the evaporation of droplet was significantly accelerated. As shown in Fig. 14 (b), at time t = 10 s, 91.5% of the exhaled droplets had become airborne, among which 87% were smaller than 10 μm. Correspondingly, the mass fraction of inhalable pathogens sharply increased to 5.05 × 10⁻⁴ with 4.89 × 10⁻⁴ being carried by the droplets/nuclei smaller than 10 μm. Compared with the 2.18 × 10⁻³ mass fraction yielded from the medium (50%) relative humidity (Case 3), the 5.05 × 10⁻⁴ mass fraction predicted with the low (10%) relative humidity (Case 9) was more than 2 times larger. Given that the morbidity of many respiratory diseases is strongly related to the exposure dose [28], it is expected that the elevated mass concentration of the inhalable pathogen in the air could increase the probability of infection, particularly increase the risk of lower respiratory tract infections.
may also give a useful clue to the mystery why influenza always breaks out in winters [3,29] because of the lower relative humidity in winters.

4. Conclusions

A multi-component Eulerian-Lagrangian model was presented in this study to model the evaporation and dispersion of cough droplets in quasi-quiescent air. The model features a water vapor transport equation which is capable of taking into account the inhomogeneous humidity field. A number of computations with various cough and environmental conditions were conducted to evaluate the critical parameters affecting the evaporation and dispersion of cough droplets. The conclusions arising from this study are as follows:

1) The inhomogeneous humidity field induced by vapor exhalation and droplet evaporation has a strong effect on the characteristics of droplet evaporation and dispersion. When the transport of evaporation-induced water vapor and exhaled water vapor was progressively included in the computational model, the predicted median evaporation time of the 12-μm droplets significantly increased. It was demonstrated that the exhaled water vapor can form a “vapor plume” in front of the respiratory tract opening. Despite its short life time (only a few seconds), the vapor plume is big enough to contain all the airborne droplets and significantly impedes their evaporation. Consequently, the airborne droplets were predicted to travel faster when the inhomogeneous humidity diffusion was included. Comparatively, the evaporation of droplets larger than 100 μm is insensitive to the vapor plume, probably because their travelling speed is larger than the dispersion speed of the vapor plume so that they are mostly located outside the vapor plume.

2) The mass of exhaled liquid and the ambient temperature and humidity all have their effects on the droplet evaporation rate and dispersion pattern. Comparatively, the ambient humidity plays a critical role.

3) Evaporation causes the droplet sizes to decrease, making some free-falling droplets become airborne and some airborne droplets become small enough to penetrate into the lower airways. Consequently, both the number density of airborne droplets/nuclei and the mass concentration of inhalable pathogens can be significantly increased, resulting in higher infection risks, particularly higher infection risks of the lower respiratory tracts.

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