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

Xiangdong Li[a], Yidan Shang[a], Yihuan Yan[a], Lin Yang[a], Jiyuan Tu[a,b,*]

[a] School of Engineering, RMIT University, PO Box 71, Bundoora, Vic 3083, Australia
[b] Key Laboratory of Ministry of Education for Advanced Reactor Engineering and Safety, Institute of Nuclear and New Energy Technology, Tsinghua University, PO Box 1021, Beijing 100086, China

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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 inhalable 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 modelling 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.

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 $d_{d,e}$ is correlated to its initial diameter $d_{d,0}$ by Ref. [9].

* Corresponding author. School of Engineering, RMIT University, PO Box 71, Bundoora, Vic 3083 Australia.
E-mail address: jiyuan.tu@rmit.edu.au (J. Tu).

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$$d_{d,e} = \left(\frac{C_{nv}}{\rho_{nv}}\right)^{1/3} d_{d,0} \tag{1}$$

A common estimation of the droplet density and initial concentration of non-volatile compounds is $\rho_{nv} = 1000$ kg/m^3 and $C_{nv} = 1.8\%$ [8], which results in an equilibrium diameter of $d_{d,e} = 0.262 d_{d,0}$. 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 μm needed only 0.07 s to reach its equilibrium diameter in dry air (0% relative humidity, RH) while a 100-μm 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

$$\varphi_m = f_a \varphi_a + f_v \varphi_v \tag{2}$$

where, the subscripts m, a and v denote the air-vapor mixture, dry air and water vapor, respectively. φ represents a property parameter ($\varphi = \rho, \mu, \lambda, c_p$, 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

$$\frac{\partial}{\partial t}(\rho_m f_a) + \nabla\cdot(\rho_m f_a \vec{U}_m) = 0 \tag{3}$$

$$\frac{\partial}{\partial t}(\rho_m f_v) + \nabla\cdot(\rho_m f_v \vec{U}_m - \rho_m D_k(\nabla f_v)) = S_v \tag{4}$$

where, $\vec{U}_m$ is the mass-averaged mixture velocity. S_v is the mass source of water vapor due to droplets evaporation. D_k 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

$$\frac{\partial}{\partial t}(\rho_m \vec{U}_m) + \nabla\cdot(\rho_m \vec{U}_m \vec{U}_m - \mu_m(\nabla \vec{U}_m + (\nabla \vec{U}_m)^T)) = S_{Buoy} + \vec{F}_{md} - \nabla p \tag{5}$$

$$\frac{\partial}{\partial t}(\rho_m H_m) + \nabla\cdot(\rho_m \vec{U}_m H_m - \nabla(\lambda_m T_m)) = Q_{md} \tag{6}$$

where, S_{Buoy} is the momentum source due to buoyancy, $\vec{F}_{md}$ is the interfacial forces acting on the droplet interfaces, ∇P is the pressure gradient, H_m is the mixture enthalpy, T_m is the mixture temperature and Q_{md} 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

$$Q_{md} = \sum_{i=1}^{N} q_{md} = \sum_{i=1}^{N} [\pi d_d^2 h_{md}(T_m - T_d)] \tag{7}$$

where, d_d is the droplet diameter, T_d is the droplet temperature and h_{md} is the interfacial heat transfer coefficient estimated according to Ranz and Marshall [20].

$$Nu_d = \frac{h_{md} d_d}{\lambda_m} = 2 + 0.6\,\mathrm{Re}_d^{0.5}\mathrm{Pr}_m^{1/3} \tag{8}$$

where, Re_d and 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 $\vec{F}_{Buoy}$ and drag force $\vec{F}_D$ are considered and the equation of droplet motion is defined by

$$m_d \frac{d\vec{U}_d}{dt} = \vec{F}_{Buoy} + \vec{F}_D \tag{9}$$

$$\vec{F}_{Bouy} = \frac{\pi d_d^3}{6} = (\rho_d - \rho_m)\vec{g} \tag{10}$$

$$\vec{F}_D = \frac{C_D}{2}\frac{\pi d_d^2}{4}\rho_m |\vec{U}_d - \vec{U}_m|(\vec{U}_d - \vec{U}_m) \tag{11}$$

where, $\vec{U}_d$ is the droplet velocity.