# Numerical Study of Cough Droplets Evaporation and Dispersion in an Indoor Environment using the Multi-component Eulerian-Lagrangian approach

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#### Abstract

The research objective is a numerical study of cough droplets evaporation and dispersion in an indoor environment using the multi-component Eulerian-Lagrangian approach to understand the basic aerosol science of SARS-CoV-2-laden droplets spread through the quasi-quiescent air. These results revealed that the smaller droplet evaporates faster than the larger droplet over a considerable time difference due to the enlarged specific surface area for heat and mass transfer, whereas the higher relative humidity of the air plays an important role to increase evaporation time. It was found that the higher temperatures were affected to accelerate the mass transfer to be fast evaporating and the initial droplet diameter  $\leq 120 \ \mu m$  was completely evaporated until became droplet nuclei because the droplets were floating and dispersing still within the domain. The evaporation time called the falling time of initial droplet diameter  $\geq 140 \ \mu m$  was canceled in a short time due to the large droplets falling to trap the bottom wall boundary. Moreover, the lowest temperature has a longer evaporation time and the least falling time, and the shortest horizontal distance because the residual droplet mass is greater than others.

*Keywords:* SARS-CoV-2-laden cough droplets, Cough droplets, Evaporation, Droplet nuclei, Multi-component Eulerian-Lagrangian model

### 1. Introduction

It is now known for certain that the SARS-CoV-2 virus that is contained within the droplets of COVID-19 can be transmitted through the aerosols produced when affected people breathe or sneeze. <sup>[1]</sup> Large droplets are produced from saliva during activities such as sneezing and wheezing, and microscopic droplets are created by coating the mucous membranes of the airways and the vocal cords. The larger particles can sometimes be seen with the unaided eye, but the smaller ones are usually obscured. Depending on the ventilation in the region, the droplets may transport contagious agents such as pathogens or viral groups into the air, which may lead to the spread of infectious illnesses. In most cases, the droplet containing pathogens is generated when a person who is affected coughs or sneezes, which is the process that causes sneezing fog with numerous droplets. The force of gravity caused enormous droplets to fall to the ground in a relatively brief amount of time. The residual particles are known as droplets nuclei or aerosols and have the ability to transfer pathogens over longer distances. Small droplets have the ability to remain airborne for extended periods of time, but they have a tendency to dissipate quickly in dry air.<sup>12, 3]</sup> Additional particle nuclei that are kept in the air by a combination of buoyancy and temperature forces.<sup>[4]</sup> Suspend the droplet after it has been adsorbed on the small solid particles in order to progressively generate bioaerosol particles in the droplet nucleus. As far back as the 1940s. Duguid (1946) studied the size of droplets from speaking, coughing and sneezing through microscopic measurements and found that the droplet diameter ranged from 1 µm to 2,000 µm and that 95% of the droplets are smaller than 100 μm.<sup>[5]</sup> In a study by Kwak et al., saliva evaporates slowly compared to water droplets due to the attraction of ions/proteins in the saliva.<sup>[6]</sup> Additionally, droplets on the ground may rise into the air again because of evaporation.<sup>[7]</sup> For droplets ranging in diameter from 1 to 1,000 µm, wells [8] and Xie et al.<sup>[9]</sup> compared the time for

complete evaporation of isolated droplets to their settling time and reported that drops with diameter  $d > 100 \mu m$  settle in liquid form to the ground in less than one second.

The computational fluid dynamics (CFD) **analysis** should be achieved in a satisfactory agreement, which must predict the evaporation and dispersion of the droplets that **convert** into the solid droplet nuclei. Since the outbreak of COVID-19, most scientists have focused their attention on predicting the respiratory droplets produced by people infected with the virus to different areas and environments using experiments and numerical study. The relevant literature contains experimental studies and numerical studies using Euler-Euler or Euler-Lagrange based models.<sup>[1, 7, 9-19]</sup> Several **studies have** neglected the mechanism of evaporation became to nuclei (aerosol) of the cough droplets, which may limit the validity of droplet nuclei trajectory predictions. However, respiratory droplets are composed of water and a small number of non-volatile compounds that can represent viral load.

In the literature review, only a few papers propose the numerical model to investigate the water in the droplet evaporates of exhalation and cough in the various ambient conditions and ultimately leaves the non-volatile components into the solid droplet nuclei as follows. Chen and Zhao employ a numerical model to investigate the dispersion characteristics of human exhaled droplets in ventilation rooms.<sup>[20]</sup> Yang et al. investigated the impact of initial droplet size to simulate the dispersion process of the droplets with an initial diameter of 10 µm and 100 µm, and gaseous contaminant in a unidirectional ventilated protective isolation room and studied the droplets dispersion and cross-transmission with different sizes.<sup>[21]</sup> Li et al. proposes the modeling of evaporation of cough droplets in inhomogeneous humidity fields using the multi-component Eulerian-Lagrangian approach to investigate the cough droplet transport and size change dynamics in a static ambient air condition.<sup>[22]</sup> The multi-component Eulerian-Lagrangian model was employed to realize the mechanistic modelling of droplet evaporation process of the thermal effect of the human body on the evaporation of the cough droplets in an enclosed space.<sup>[23]</sup> Calmet et al. used a highly resolved mesh of large eddy simulation to capture the multiphase turbulent buoyant cloud with suspended droplets produced by a cough. The cough droplets' dispersion was subjected to thermal gradients and evaporation and allowed to disperse between two humans standing 2 m apart.<sup>[24]</sup>

In this study, droplet evaporation and dispersion are provided by using numerical modeling to understand the basic aerosol science of SARS-CoV-2-laden droplets spread through the air of indoor environment as quasi-quiescent air. Numerical modeling can be extended to provide high resolution on the transport of infected aerosols and prediction of their accumulation from the human respiratory system. To estimate the RNA load of SARS-CoV-2 in a room or enclosed space. To further understand viral infection, replication, and disease pathogenesis in the near future and to better prepare for the post-epidemic phase and have a high chance of resuscitation. Although, an isolation room, the pressurization specification can be achieved by exhausting at least 15% more air than the supply air with 6-12 ACH<sup>[25, 26]</sup> but for an indoor environment, it is not ensured for guarantees a reduction of viral transmission from cough droplets. Therefore, to study the mitigation strategies for reducing viral transmission in the ventilation design for various indoor environments, the generation of solid droplet nuclei from coughing, sneezing, and talking has inspired the use of numerical simulation, which investigates the droplet-laden cough jet with the reality of the spread of pathogens. Consequently, this research objective proposed the numerical study with the multi-component Eulerian-Lagrangian approach to study droplet evaporation and dispersion in quiescent air. The size reduction until became droplet nuclei and trajectory of the cough droplets were predicted to study the influent temperatures with specific relative humidity.

### 2. Governing Equations

In the governing equations, the RNG k- $\varepsilon$  model is coupled with a Discrete Phase Model (DPM), energy equation, and species transport equation. The RNG *k*– $\varepsilon$  model can be predicted more swirls and more complex trajectories.<sup>[4, 21, 22, 25, 27]</sup> The multi-component Eulerian-Lagrangian model was applied to realize the mechanism of droplet evaporation process. The flow has two phases: the carrier phase (air) and the discrete phase (droplets and droplet nuclei). The carrier phase is modeled by Eulerian model whereas the discrete phase is modeled by Lagrangian model. **Expression for** continuity, momentum, energy, species, turbulent model, DPM model are as follows <sup>[28]</sup>:

$$\frac{\partial \rho}{\partial t} + \nabla . \left( \rho \vec{v} \right) = S_m \tag{1}$$

where  $\rho$  and  $\vec{v}$  are gas density and velocity, and  $S_m$  is mass source term.

$$\frac{\partial}{\partial t}(\rho \vec{v}) + \nabla .(\rho \vec{v} \vec{v}) = -\nabla p + \nabla .(\vec{\tau}) + \rho \vec{g} + U_p S_m + \vec{F}_{gp}$$
(2)

where p is the static pressure,  $\bar{\tau}$  is the stress tensor (described below),  $\rho \vec{g}$  is the gravitational body force.  $\vec{F}_{gp}$  is sum of the forces exerted by particles on the gas phase.

$$\stackrel{=}{\tau} = \mu \left[ \left( \nabla \vec{v} + \nabla \vec{v}^T \right) - \frac{2}{3} \nabla . \vec{v} I \right]$$
(3)

where  $\mu$  is the molecular viscosity, *I* is the unit tensor, and the second term on the right hand side is the effect of volume dilation.

$$\frac{\partial}{\partial t} \left( \rho \left( e + \frac{v^2}{2} \right) \right) + \nabla \left( \rho v \left( h + \frac{v^2}{2} \right) \right) = \nabla \left( k_{eff} \nabla T - \sum_j h_j \vec{J}_j + \vec{\tau}_{eff} \cdot \vec{v} \right) + S_h$$
(4)

where  $k_{eff}$  is the effective conductivity,  $\vec{J}_{j}$  and is the diffusion flux of species, j. The first three

terms on the right-hand side of Eq.4 represent energy transfer due to conduction, species diffusion, and viscous dissipation, respectively. The  $h_j$  is the part of enthalpy that includes only changes in the enthalpy due to specific heat.  $S_h$  includes volumetric heat sources that you have defined and the heat generation rate from chemical reactions.

$$\frac{\partial}{\partial t} (\rho Y_i) + \nabla . (\rho \vec{v} Y_i) = -\nabla . \vec{J}_i + R_i + S_i$$
(5)

This choose to solve conservation equations for chemical species due to fluid composition of human raspatory and air surrounding are moist air and CO<sub>2</sub>, Ansys Fluent predicts the local mass fraction of each species,  $Y_i$ , through the solution of a convection-diffusion equation for the  $i^{th}$  species that is mass fraction of vapour in humid gas.

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j}\left(\alpha_k \mu_{eff} \frac{\partial k}{\partial x_j}\right) + G_k + G_b + S_k \tag{6}$$

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \frac{\partial}{\partial x_i}(\rho\varepsilon u_i) = \frac{\partial}{\partial x_j}\left(\alpha_{\varepsilon}\mu_{eff}\frac{\partial\varepsilon}{\partial x_j}\right) + C_{1\varepsilon}\frac{\varepsilon}{k}(G_k + C_{3\varepsilon}G_k) - C_{2\varepsilon}\rho\frac{\varepsilon^2}{k} - R_{\varepsilon} + S_{\varepsilon}$$
(7)

where  $\rho$  is fluid density, k is turbulence kinetic energy,  $\varepsilon$  is the turbulence dissipation rate,  $u_i$  is velocity components,  $\alpha_k$  and  $\alpha_{\varepsilon}$  are inverse effective Prandtl numbers for k and  $\varepsilon$ ,  $\mu_{eff}$  is effective viscosity,  $C_{1\varepsilon}$ ,  $C_{2\varepsilon}$  and  $C_{3\varepsilon}$  are turbulent model constants, these values, used by default in Ansys Fluent, are  $C_{1\varepsilon}=1.42$  and  $C_{2\varepsilon}=1.68$ ,  $R_{\varepsilon}$  is main difference between the RNG k- $\varepsilon$  and standard k- $\varepsilon$  models lies in the additional term in the  $\varepsilon$  equation,  $S_k$  and  $S_{\varepsilon}$  are user-defined source terms.

Modeling turbulent production in the k- $\varepsilon$  models, the term  $G_k$  represents the generation of turbulence kinetic energy due to the mean velocity gradients, representing the production of

turbulence kinetic energy, is modeled identically for RANS models. From the exact equation for the transport of k, this term is defined as:

$$G_k = -\rho \overline{u_i u_j} \frac{\partial u_j}{\partial x_i}$$
(8)

When a nonzero gravity field and temperature gradient are present simultaneously,  $G_b$  is the generation of turbulence kinetic energy due to buoyancy, this is given by

$$G_b = \beta g_i \frac{\mu_t}{\Pr_t} \frac{\partial T}{\partial x_i}$$
(9)

where  $Pr_t$  is the turbulent Prandtl number for energy, the default value is 0.85. The coefficient of thermal expansion,  $\beta$ , is defined as

$$\beta = -\frac{1}{\rho} \left( \frac{\partial \rho}{\partial T} \right)_{p} \tag{10}$$

The constitutive relationship between air temperature, pressure and density is given by the ideal gas law (such model is sufficient because of small humidity of the gas involved in the considered multiphase flow):

$$p = \frac{\rho}{M} RT \tag{11}$$

where R is universal gas constant and M is molecular weight of the gas phase.

To track the trajectories and other valuable parameters of cough droplets and particles, a DPM model based on Lagrangian formulation is utilized. This force balance equates the particle inertia with the forces acting on the particle, and can be written as

$$m_p \frac{d\vec{u}_p}{dt} = m_p \frac{\vec{u} - \vec{u}_p}{\tau_r} + m_p \frac{\vec{g} \left(\rho_p - \rho\right)}{\rho_p} + \sum \vec{F}_i$$
(12)

where  $m_p$  is the particle mass,  $\vec{u}$  is the fluid phase velocity,  $\vec{u}_p$  is the particle velocity,  $\rho$  is

the fluid density,  $\rho_p$  is the density of the particle,  $\sum \vec{F}_i$  is an additional force *i* denotes particle *i*,  $m_p (\vec{u} - \vec{u}_p) / \tau_r$  is the drag force,  $F_D$ , and  $\tau_r$  is droplet or particle relaxation time calculated by:

$$\tau_r = \frac{\rho_p d_p^2}{18\mu} \frac{24}{C_d \operatorname{Re}}$$
(13)

here,  $\mu$  is the molecular viscosity of the fluid,  $d_p$  is the particle diameter, for smooth particles the drag coefficient,  $C_d$ , can be taken from

$$C_d = a_1 + \frac{a_2}{\text{Re}} + \frac{a_3}{\text{Re}^2}$$
(14)

where  $a_1$ ,  $a_2$ , and  $a_3$  are constants that apply over several ranges of Reynolds number (Re) that is the relative, which is defined as

$$\operatorname{Re} = \frac{\rho d_p \left| \vec{u}_p - \vec{u} \right|}{\mu} \,. \tag{13}$$

In Eq. 12 incorporates additional forces in the particle force balance that can be important under special circumstances. The first of these is the "virtual mass" force, the force required to accelerate the fluid surrounding the particle.  $C_{vm}$  is the virtual mass coefficient. This force can be written as

$$\vec{F}_{i,vir} = C_{vm} m_p \frac{\rho}{\rho_p} \left( \vec{u}_p \nabla \vec{u} - \frac{d\vec{u}_p}{dt} \right)$$
(15)

Small particles suspended in a gas that has a temperature gradient experience a force in the direction opposite to that of the gradient. This phenomenon is known as thermophoresis force,  $\vec{F}_T$ . Ansys Fluent can optionally include a thermophoretic effect on particles in the additional force

$$\vec{F}_T = -D_{T,p} \frac{1}{T} \nabla T \tag{16}$$

where  $D_{T,p}$  is the thermophoretic coefficient. You can define the coefficient to be constant, polynomial, or a user-defined function, or you can use the form suggested by Talbot:

$$D_{T,p} = \frac{6\pi d_p \mu^2 C_s \left(K + C_t Kn\right)}{\rho \left(1 + 3C_m Kn\right) \left(1 + 2K + 2C_t Kn\right)}$$
(17)

where Kn is Knudsen number  $(2\lambda/d_p)$  that this expression assumes that the particle is a sphere,  $\lambda$  is mean free path of the fluid,  $K = k/k_p$ , k is fluid thermal conductivity based on translational energy only = (15/4)  $\mu R$ , T is local fluid temperature,  $\mu$  is fluid viscosity,  $C_m = 1.14$ ,  $C_s = 1.17$ , and  $C_t = 2.18$ .

The Saffman's lift force,  $\vec{F}_{Saffman}$ , or lift due to shear, can also be included in the additional force term as an option. The lift force used is a generalization of the expression provided by Saffman:

$$\vec{F}_{Saffman} = m_p \frac{2K v^{1/2} \rho d_{ij}}{\rho_p d_p \left( d_{lk} d_{kl} \right)^{1/4}} \left( \vec{u} - \vec{u}_p \right)$$
(18)

where K and  $d_{ij}$  is the deformation tensor. This form of the lift force is intended for small particle Reynolds numbers and is recommended only for sub-micron particles.

Brownian motion arises because of individual collisions between molecules and particles. These collisions will lead to a sort of particle diffusion. Brownian motion is only important for sub-micron particles. Since only a small fraction of the cough droplet particles have a diameter in the order of 1  $\mu$ m the Brownian motion was considered superfluous for the simulations. The modeling of Brownian motion resembles that of turbulent dispersion. Brownian motion is modeled as white noise. The force components are modeled with the product of a Gaussian distributed random number and the square root of the spectral intensity,  $S_{n,ij}$  given by:

$$S_{n,ij} = S_0 \delta_{ij} \tag{19}$$

where  $\delta_{ii}$  is the Kronecker delta function, and

$$S_0 = \frac{216vk_BT}{\pi^2 \rho d_p^5 \left(\frac{\rho_p}{\rho}\right)^2 C_c}$$
(20)

where T is the absolute temperature of the fluid, v is the kinematic viscosity,  $C_c$  is the Cunningham correction, and  $k_B$  is the Boltzmann constant. Amplitudes of the Brownian force components are of the form

$$F_{b_i} = m_p \zeta_i \sqrt{\frac{\pi S_0}{\Delta t}}$$
(21)

where  $\zeta_i$  are zero-mean, unit-variance-independent Gaussian random numbers. The amplitudes of the Brownian force components are evaluated at each time step. The energy equation must be enabled for the Brownian force to take effect. Brownian force is intended only for laminar simulations. The drag function is expressed as:

$$F_{D}\left(u-u_{p}\right) = \frac{\mu}{p_{d}d_{p}^{2}} \frac{18C_{D}\operatorname{Re}}{24}\left(u-u_{p}\right)$$
(22)

for sub-micron particles, a form of Stokes' drag law is available. In this case, is defined as

$$F_D = \frac{18\mu}{d_p^2 \rho_p C_c},\tag{23}$$

the factor is the Cunningham correction to Stokes' drag law, which you can compute from

$$C_{c} = 1 + \frac{2\lambda}{dp} \left( 1.257 + 0.4e^{-(1.1d_{p}/2\lambda)} \right)$$
(24)

where,  $\lambda$  is the molecular mean free path.

The dispersion of particles due to turbulence in the fluid phase, this work was predicted using

the stochastic tracking model. Ansys Fluent uses a stochastic method (random walk model) to determine instantaneous gas velocity. In the Discrete Random Walk (DRW) model, the fluctuating velocity components are discrete piecewise constant functions of time. Their random value is kept constant over an interval of time given by the characteristic lifetime of the eddies.

Discrete phase modeling can model the reacting particles or droplets and the effect on continuous phases can be examined. The relationship of heat and mass transfer, known as the "law", is contained in Ansys Fluent and the physical model used in multi-component particle definition (Law 7). The particle mass m is the sum of the masses of the components

$$m = \sum_{i} m_{i} \tag{25}$$

The density of the particle can be either constant, or volume-averaged:

$$\rho_p = \left(\sum_i \frac{m_i}{m\rho_i}\right)^{-1} \tag{26}$$

The multicomponent droplet vaporization rate is calculated as the sum of the vaporization rates of the individual components. For the diffusion-controlled vaporization model, the vaporization rate of component is given by

$$\frac{dm_i}{dt} = A_p M_w k_{c,i} \left( C_{i,s} - C_{i,\infty} \right)$$
(27)

when the rate of vaporization is slow, it can be assumed to be governed by gradient diffusion, with the flux of droplet vapor into the gas phase related to the difference in vapor concentration at the droplet surface and the bulk gas:

$$N_i = k_{c,i} \left( C_{i,s} - C_{i,\infty} \right) \tag{28}$$

where  $m_i$  is mass of component *i* in droplet (kg),  $k_{c,i}$  is mass transfer coefficient of component *i* (m/s) and  $N_i$  is molar flux of vapor (kmol/m<sup>2</sup>-s),  $A_p$  is droplet surface area (m<sup>2</sup>),

 $C_{i,s}$  and  $C_{i,\infty}$  are concentration of species at the droplet surface and the bulk, respectively (kmol/m<sup>3</sup>).

The concentration of vapor at the droplet surface is evaluated by assuming that the partial pressure of vapor at the interface is equal to the saturated vapor pressure,  $p_{sat}$ , at the droplet temperature,  $T_p$ :

$$C_{i,s} = \frac{p_{sat}(T_p)}{RT_p}$$
(29)

where *R* is the universal gas constant.

The concentration of vapor in the bulk gas is known from solution of the transport equation for species *i* as:

$$C_{i,\infty} = X_i \frac{p}{RT_{\infty}}$$
(30)

where  $X_i$  is the local bulk mole fraction of species *i*, *p* is the local pressure, and  $T_{\infty}$  is the local bulk temperature in the gas. The mass transfer coefficient in Eq.22 is calculated from the Sherwood number correlation:

$$Sh_{AB} = \frac{k_c d_p}{D_{i,m}} = 2.0 + 0.6 \operatorname{Re}_d^{1/2} Sc^{1/3}$$
(31)

where  $D_{i,m}$  is diffusion coefficient of vapor in the bulk (m<sup>2</sup>/s), Sc is the Schmidt number  $(\mu / \rho D_{i,m})$ , and  $d_p$  is particle (droplet) diameter (m). While for the convection/diffusion-controlled model, it is given by:

$$\frac{dm_i}{dt} = A_p k_{c,i} \rho \ln\left(1 + B_{m,i}\right) \tag{32}$$

where  $\rho$  is gas density (kg/m<sup>3</sup>),  $M_w$  is molecular weight of species, *i*, and  $B_{m,i}$  is the Spalding

mass number.

$$B_m = \frac{Y_{i,s} - Y_{i,\infty}}{1 - Y_{i,s}}$$
(33)

where  $Y_{i,s}$  is vapor mass fraction at the surface,  $Y_{i,\infty}$  is vapor mass fraction in the bulk gas. The energy equation is written for the multicomponent particle as follows:

$$m_p c_p \frac{dT}{dt} = h A_p \left( T_{\infty} - T_p \right) + \sum_i \frac{dm_i}{dt} \left( h_{vap,i} \right)$$
(34)

where  $dm_i/dt$  is computed from Eq.27 and 32,  $h_{vap,i}$  is latent heat of vaporization for component *i*, *h* is heat transfer coefficient for the diffusion-controlled vaporization model as follows:

$$Nu = \frac{hd_p}{k_{\infty}} = 2.0 + 0.6 \operatorname{Re}_d^{1/2} \operatorname{Pr}^{1/3},$$
(35)

where Nu is the Nusselt number,  $k_{\infty}$  is thermal conductivity of the continuous phase (W/m-K), Re<sub>d</sub> is Reynolds number based on the particle diameter and the relative velocity. The exchange of mass and energy between liquid droplets of cough or sneeze and the surrounding gases was calculated droplet by droplet. After the temperature of each droplet is calculated, the amount of vaporized liquid is added to the mesh cell and the gas temperature in the cell is balanced according to the energy exchange between the droplet and the surroundings.

To simulate evaporation of water into so-called solid particles, multi-component particles are used in conjunction with a user-defined function (UDF). Multi-component particles can inject particles containing more than one substance, such as saliva and viruses. However, with the Ansys Fluent program, only liquid particles can be represented as multi-components. Hence, it is necessary to create a multi-component particle consisting of water and additional liquids later to further change the liquid properties and to later represent real solids. In this simulation, the cough droplets were assumed by using droplets of two mass fraction evaporating species as 98.2% water and 1.8 % urea water as density of 1,000 kg/m<sup>3</sup>, the water was determined to be vaporizing and the urea water not-vaporizing. From heat and mass transfer relationships, the evaporation of the species in the droplets can be seen and the reduction of droplet diameter until the final size can be observed.

#### **3.** Introduction Geometry, mesh generation, and boundary conditions

The droplet evaporation and dispersion were studied by using numerical simulations to understand the basic aerosol science of SARS-CoV-2-laden droplets spread through the air in an indoor environment. This methodology begins with a review of the relevant literature to search for numerical models that can predict the behavior of droplet evaporation to droplet nuclei so-called solid aerosol. Due to the limitation of the HPC license on Ansys Fluent, the computational domain of cuboid space in front of a coughing person's mouth was assumed using the 2D model with the geometry of 4 m-length and 3 m-height, as shown in Fig.1. The geometry model was divided into two zones, so-called near mount zone and the rest zone to assign different grid sizing. The geometry domain was discretized using structured hexahedral grids with very fine mesh applied at the near mount zone and rest zone defined as coarse mesh.

The center of the mouth is strictly placed at 2.0 m in vertical distance of the left-hand side of the domain. The inlet boundary condition has a hydraulic diameter of 0.02 m, which represents the human mouth opening for coughing as assigned the velocity, the temperature, and humidity with same environment air. The coughing velocity can be assigned as velocity constant of cough jet and pulse of single cough. The right-hand side of the domain was set as a pressure outlet with zero-gauge pressure, which considered the ambient conditions as the air temperature and humidity. The

non-slip boundary conditions have been used for all other walls where isothermal condition was assumed. The data in boundary conditions of each computational case are listed in Table 1.



**Fig. 1** Schematic two-dimensional (axisymmetric) view of the computational domain including the boundary conditions for the case of caught droplet in static ambient air condition and computational grid.

Case No.	Inlet: Ve $U_0 = 10$	elocity inl [m/s]	et	Ambient	conditions	Outlet: Pressure	outlet	Wall: Adiabatic wall
	$T_{in}(^{\circ}\mathrm{C})$	RH(%)	U <sub>0</sub> [m/s]	$T_{\infty}$ (°C)	RH(%)	$T_{\infty}$ (°C)	RH(%)	DPM
1	25	0	10	25	0	25	0	Trap
2	25	0	Pulse	25	0	25	0	Trap
3	25	60	10	25	90	25	90	Trap
4	15	60	10	15	60	18	60	Trap
5	25	60	10	25	60	25	60	Trap

Table 1 Boundary conditions of the parametric study cases

6	35	60	10	35	60	35	60	Trap
7	45	60	10	45	60	45	60	Trap

Generally, the human cough is a variable flow rate. However, by integrating the flow rate profile along the time axis we obtain an average velocity value of 10 m/s. <sup>[29, 30]</sup> Therefore, the variable flow rate of the coughing jet at an average velocity of 10 m/s was prescribed for the air leaving the mouth in the inlet boundary condition. For pulse of a single cough was prescribed by the velocity at 10 m/s within 0.5 s.

The first step was model geometry and grid, we used the design modeler and mesh using the Ansys Workbench program. For physical setup and simulations, the governing equations were discretized based on a finite-volume method and solved using the commercial CFD code of Ansys Fluent software. The multi-component Eulerian-Lagrangian model was applied to realize the droplet evaporation process, in which the RNG *k*- $\varepsilon$  model was coupled with the DPM model, energy equation, and species transport equation. The DPM model is adopted to calculate the evaporation and transmission process of droplets in the continuous air background, which is reasonable as the expelled saliva/phlegm droplets are assumed to be composed of 98.2% water and 1.8% as urea-water with the same density as not-vaporizing. The heat and mass exchanges exist between the liquid droplet surface and the ambient air. The time step was 0.01 s for all simulation periods.

Table 2	Inree	mesnes	usea	ın	the	gria	inde	pendei	nce te	est

Mesh No.	Element size at	Element size at near	Element size at rest	Total
	inlet (mm)	mount zone (mm)	zone (mm)	elements
Mesh 1	5	10	20	33,199
Mesh 2	5	5	20	43,255
Mesh 3	5	5	10	131,136

The three different meshes called Mesh 1, Mesh 2, and Mesh 3 were generated to find out the

least required amount of meshes. The mesh sizes are divided into 3 parts. The mesh size of inlet BC is 5 mm. The mesh size of the near mount zone and rest zone are particularly adjusted by 5 to 20 mm, which mesh is generated as 33,199, 43,255, and 131,136 elements, respectively (see Table 2). The velocity inlet BC of case 1 is cough jet and case 2 is the pulse of a single cough in which the temperature of dry air (RH = 0%) and droplet is 25 °C. The droplet evaporation with an initial diameter of 10, 50, and 100  $\mu$ m are calculated to reach their equilibrium diameters using the simulation periods of 10 s. The DPM injections are prescribed by the surface released at inlet BC, in which the droplets are injected by 4 particles per time step and every 0.01 s until 10 s for cough jet to always report a diameter reduction with the current position of particle tracks and for until to 0.5 s of for pulse of a single cough. For the pulse of a single cough, the droplets are injected by 4 particles per time step and every 0.01 s until 0.5 s.

Case 3 is the validation process, in which the predicted time-dependent droplet diameter (solid lines) is compared against the reference work [23]. The boundary conditions are set as the evaporation of droplets falling freely in quiescent air, according to the literature paper, which two single droplets sizes (10 and 100  $\mu$ m) and very small droplet mass flow rates (5.24×10<sup>-11</sup> kg/s for the 10- $\mu$ m droplets and 5.24×10<sup>-8</sup> kg/s for the 100- $\mu$ m droplets, respectively) are used to match the computational conditions of the reference work. The velocity inlet BC is cough jet, which assumed the droplets are released with a time interval of 0.01 s until 100 s. The computations are conducted with a constant temperature of air and droplets of 25 °C. The relative humidity fields were changed from 0% became 90% respectively.

In cases 4 to 7, the relative humidity 30%–60% is quite suitable for most residents [33], but virus survival in droplets is determined at 60% relative humidity. Therefore, the size reduction until became droplet nuclei and trajectory of the cough droplets were predicted to study the influent

temperatures with specific relative humidity at 60% RH. The assumptions of air temperature and relative humidity of the inlet and environment are the same because the exhaled air is more dilute. The different temperature is 15, 25, 35, and 45 °C that species mass fraction of water vapor and air density follow in Table 3. The different initial droplet diameter, i.e., 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 120, 140, 150, 160, 175, 200, 225, 250, 275, and 300 µm, are injected with the same velocity of 10 m/s, and the injection frequency is 0.01 s for the simulation periods of 35 s. The droplets will be trapped when they contact the wall or fall onto the ground.

 $T(^{\circ}C)$ RH(%) Species Mass Fraction Density (kg/m<sup>3</sup>) 1.207 15 60 0.00631 25 60 0.01175 1.175 35 60 0.02099 1.131 45 60 0.03610 1.086

<b>Table 5</b> the air properties of mass fraction of species and density
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## 4. Results and discussion

#### 4.1 Mesh independent



Fig. 2 Effect of grid independent on the droplet diameter shrinks over time of varying droplet

sizes as 10, 50 and 100  $\mu$ m in dry air ( $T_p = 25 \,^{\circ}\text{C}$ ,  $T_{\infty} = 25 \,^{\circ}\text{C}$ , RH = 0%,  $U_0 = 10 \,\text{m/s}$ ).

The simulation results of Case 1 and Case 2, three different meshes (see Table 2) were generated and the evaporation in dry air of droplets with initial diameters of 10, 50, and 100 µm were calculated to find out the least required amount of meshes. The mesh independent was achieved at the number of droplet trajectories was also analyzed. It found that when the mesh number was larger than 33,199. Fig. 2 shows that the results of the three meshes almost overlap with each other. Moreover, Fig.3 shows droplet suspension patterns at different time stations of Case 2 of varying droplet sizes in dry air. Some small differences exist probably due to the occasionality of numerical simulation. Thus, the grid independence of meshes has been verified and the smallest mesh (Mesh 2) is used in the following simulations.



**Fig. 3** Effect of mesh independent on droplet suspension patterns at different time stations of Case 2 of varying droplet sizes as 10, 50 and 100  $\mu$ m in dry air ( $T_p = 25 \,^{\circ}\text{C}$ ,  $T_{\infty} = 25 \,^{\circ}\text{C}$ , RH = 0%, and  $U_0$ 

= 10 m/s).

#### 4.2 Validation results

The predicted time drop diameter (solid line) was compared with the theoretical calculation (marker) by Li et al.,<sup>[22]</sup> as shown in Fig. 4. There was a satisfactory tendency between the numerical results of this study and the validation data that the literature referenced for both the initial droplet size and the relative humidity of the air. The figure also reveals that droplet evaporation is sensitive to both parameters (initial size and relative humidity). First, the evaporation rate is greatly affected by droplet size. Smaller droplets evaporate faster than larger droplets over a considerable time difference due to the enlarged specific surface area for heat and mass transfer. Second, the relative humidity of the air plays an important role. The relative humidity was changed from 0% to 90%, the evaporation time to equilibrium diameter of droplets nuclei increases dramatically from 0.075 s to 0.55 s for 10 µm droplets and from 6.03 seconds to 33.4 seconds.





humidity ( $T_p = 25 \degree C$ ,  $T_{\infty} = 25 \degree C$ ,  $U_0 = 10 \text{ m/s}$ )

#### 4.3 The effects of the different room temperatures

Due to some results are close together and similar. Therefor the evaporation-induced size reduction results of different droplet size, i.e., 10, 20, 30, 40, 60, 100, 120, 140, 150, 160, 175, 200, 225, 250, 275, and 300  $\mu$ m, with time-dependent are shown in Fig.5, the line colors shows the effect of different room temperature levels (blue line of 15 °C, green line of 25 °C, black line of 35°C and red line of 45 °C). In the numerical setting, we set the initial temperature of the cough droplets at 33°C, and the ambient temperature at 15, 25, 35, and 45 °C, respectively with same RH. The droplet sizes as different initial sizes were injected into the computational domain using different boundary conditions in the cases 3 to 6, respectively. The droplets are evaporated completely as long as the trajectory float in the domain, and evaporation is canceled when the droplets were trapped and escape the domain boundaries. It is found the evaporation of droplet sizes of about 10-120 µm was found that the droplets were evaporated completely until they became solid aerosols in a short time. The higher temperatures have the effect of fast evaporating until final sizes as solid aerosols about 26.2% of initial particle diameters. The evaporation of 140-300 µm droplets is canceled within 5 seconds of evaporation time due to the droplets falling to the wall boundary. The lowest temperature at 15°C was slightly longer evaporation time than higher temperatures, which the other cases have a close evaporation time.

The completed evaporation time of different droplet size for 10-120  $\mu$ m and the end of evaporation time for the bigger size were collected to plot the relation curves of evaporation time vs. initial particle diameter, and vs. final particle diameter as shown in Fig. 6. In the same figure, primary plot of curves is initial particle diameters (x-axis) versus evaporation time (y-axis) as different ambient temperatures that result found the higher the temperature has the effect to

decrease completed evaporation time for initial particle diameters of 10-120  $\mu$ m. The evaporation time was canceled in the short time for initial particle diameters 140-300  $\mu$ m, but the evaporation not completed due to the droplet particles dropped on the bottom wall boundary, which evaporation time can be called falling time. The secondary diagram is curves of final particle diameter vs. evaporation time. In the results revealed that the initial particle diameter of 10-120  $\mu$ m was completely evaporated within 5s and the initial particle diameter 140-300  $\mu$ m was not completely evaporation, which the final size has been reduced only slightly due to the droplets falling to the wall boundary.



**Fig. 5** The size reduction versus evaporation time of the droplets of different initial sizes, i.e., 10, 20, 30, 40, 60, 100, 140, 150, 160, 175, 200, 225, 250, 275, and 300  $\mu$ m of different ambient temperature (— blue line of 15 °C, — green line of 25 °C, — black line of 35 °C and — red line of 45 °C).



**Fig. 6** The evaporation time vs initial particle diameters vs final particle diameters curves of droplets at different temperatures levels.

Figure 7 show the x-y trajectories vs falling time of six different diameters droplets such as 100, 120,150, 200, 250, and 300 µm at different ambient temperatures., i.e., 15, 25, 35, and 45 °C within 35s. The y-axis of the primary plot is the vertical distance of domain height (orange line of 15 °C, gold line of 25 °C, green line of 35°C and dark orange line of 45 °C). And the y-axis of the secondary plot is the horizontal distance of domain width (red line of 15 °C, black line of 25 °C, blue line of 35°C and dark blue line of 45 °C), which the horizontal distance can be provided to evaluate the social distancing.

Fig.7a and 7b show the x-y trajectories with time-dependent of 100 and 120  $\mu$ m, it was found that droplet motion was quite difficult to determine trajectory both vertically and horizontally at any time. However, droplets were floating and dissipation in the all-around the domain, which the droplet size  $\leq$  120  $\mu$ m could be successfully evaporated to be solid aerosols.



**Fig. 7** The x-y trajectories of droplets of six different diameters at different ambient temperature, i.e., 15, 25, 35, and 45 °C, different diameter seem in the chart title.



**Fig. 8** Comparison the droplet size distributions of cough jet results with 15°C and 60% RH in quasi-quiescent air at: (a) t = 0.5 s, (b) t = 1 s, (c) t = 2 s, (d) t = 3 s, (e) t = 4s, (f) t = 5 s.



**Fig. 9** Comparison the droplet size distributions of cough jet results with 25°C and 60% RH in quasi-quiescent air at: (a) t = 0.5 s, (b) t = 1 s, (c) t = 2 s, (d) t = 3 s, (e) t = 4 s, (f) t = 5 s.



**Fig. 10** Comparison the droplet size distributions of cough jet results with 35°C and 60% RH in quasi-quiescent air at: (a) t = 0.5 s, (b) t = 1 s, (c) t = 2 s, (d) t = 3 s, (e) t = 4 s, (f) t = 5 s.



**Fig. 11** Comparison the droplet size distributions of cough jet results with 45°C and 60% RH in quasi-quiescent air at: (a) t = 0.5s, (b) t = 1 s, (c) t = 2 s, (d) t = 3 s, (e) t = 4 s, (f) t = 5 s.

The x-y trajectories as Fig.7c, the falling time of droplet size 150 µm at temperatures 15, 25, 35, and 45 °C were 3.74, 1.49, 1.57, and 1.46 s, respectively, and 0.727, 3.21, 3.82, and 3.34 m, respectively for horizontal distance. The x-y trajectories as Fig.7d, the falling time of droplet size 200 µm at temperatures 15, 25, 35, and 45 °C were 2.01, 1.02, 1.16, and 1.17 s, respectively, and 1.39, 3.01, 3.01, and 3.05 m, respectively for horizontal distance. The x-y trajectories as Fig.7e, the falling time of droplet size 250 µm at temperatures 15, 25, 35, and 45 °C were 1.38, 0.98, 1.03, and 1 s, respectively, and 2.15, 3.24, 3.24, and 3.23 m, respectively for horizontal distance. Finally, the x-y trajectories as Fig.7f, the falling time of droplet size 300 µm at temperatures 15, 25, 35, and 45 °C were 1.06, 0.91, 0.92, and 0.88 s, respectively, and 2.98, 3.69, 3.75, and 3.82 m, respectively for horizontal distance. In above results found that the lowest temperature at 15°C has a slightly longer evaporation time than higher temperatures, while the other cases have a close evaporation time. This temperature has significantly the shortest falling time and the shortest horizontal distance, in which the other cases both falling time and horizontal distance were approximately the same.

Fig. 8 to 11 show the cough droplet jet with 10 m/s from the human mouth that compare the droplet distributions of different initial diameter (every 10  $\mu$ m between 10  $\mu$ m and 160  $\mu$ m, every 25  $\mu$ m between 247  $\mu$ m and 300  $\mu$ m) of predicted results with different temperature (15°C, 25°C, 35°C, and 45°C) and same RH at 0.5 s, 1 s to 5 s in quasi-quiescent air. It can be seen that, the cough droplet jet can freely develop, and the droplets travel along with the jet flow under quasi-quiescent air in an indoor environment. The higher temperatures have to influent faster dropping and farther horizontal distances, but the lower temperature tends to more vertical distance.

### 5. Conclusion

The numerical simulation investigated cough droplet evaporation and diffusion in quiescent air and was verified by comparing the current simulation data with the data in literature. The cough droplets at 10 and 100 µm evaporate at 25 °C with air relative humidity of 0 and 90%. The evaporation time, falling time, and direction of difference diameters (i.e., 10, 20, 30, 40, 60, 100, 120, 140, 150, 160, 175, 200, 225, 250, 275, and 300 µm) of cough droplets at 15, 25, 35, and 45 °C and 60% RH are determined by the room temps. The following are the findings of this investigation:

- a) The validation results of this study were consistent with the reference data, for both initial droplet diameter at 10 μm and 100 μm and air relative humidity of 0 and 90%.
- b) The evaporation rate is greatly affected by droplet size, which the smaller droplet evaporates faster than larger droplet over a considerable time difference due to the enlarged specific surface area for heat and mass transfer.
- c) The higher relative humidity of the air plays an important role to increase evaporation time.
- d) The higher temperatures of the environment can accelerate the mass transfer to be fast evaporating than lower temperatures.
- e) The evaporation of initial droplet diameter ≤ 120 µm was completely evaporated until became droplet nuclei in a short time about 26.2% of initial diameters because the droplets were floating and dispersing still within the domain.
- f) The evaporation time or falling time of initial droplet diameter  $\geq 140 \ \mu m$  was canceled within 5 seconds due to the droplets falling to trap the bottom wall boundary.
- g) The lowest temperature at 15°C has a slightly longer evaporation time than higher

temperatures, while the other cases have a close evaporation time. This temperature has significantly the shortest falling time and the shortest horizontal distance because the residual droplet mass was greater than in the other cases, in which the other cases both falling time and horizontal distance were approximately the same.

Finally, still, there are some limitations in this work. For instance, the droplet evaporation is canceled when the droplets drop to walls because the wall film model in the DPM model is not used in the wall boundary condition. The transient processes of coughing and the three-dimension model can be worth future study.

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## **Supporting information**

Available at

# **Conflict of interest**

There are no conflicts to declare.

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