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A simplified model to estimate COVID19 transport in enclosed spaces

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Abstract. Airborne pathogen respiratory droplets are the primary route of COVID19 transmission, which are released from infected people. The strength and amplitude of a release mechanism strongly depend on the source mode, including respiration, speech, sneeze, and cough. This study aims to develop a simplified model for evaluation of spreading range (length) in sneeze and cough modes using the results of Eulerian-Lagrangian CFD model. The Eulerian computational framework is first validated with experimental data, and then a high-fidelity Lagrangian CFD model is employed to monitor various scale particles’ trajectory, evaporation, and lingering persistency. A series of Eulerian-Lagrangian CFD simulations is conducted to generate a database of bioaerosol release spectrum for the release modes in various thermal conditions of an enclosed space. Eventually, a correlation fitted over the data to offer a simplified airborne pathogen spread model. The simplified model can be applied as a source model for design and decision-making about ventilation systems, occupancy thresholds, and disease transmission risks in enclosed spaces.

1. Introduction

The primary transmission mode of COVID19 is understood to be in-person exposure to infected people’s respiratory secretions and bioaerosols expelled in various sizes [1]. Before reaching an effective vaccine, social distancing remains the inevitable defensive measure during pandemics. Maintaining a physical distance between people, as one of the means of social distancing, is enforced by many governments across the world while the essence of such stipulated measures is adapted from early pieces of evidence regarding the release and environmental persistence of SARS-CoV2 [2]. From fluid dynamics perspective, COVID19 transmission mode via respiratory airborne pathogen droplets requires a thorough investigation of droplets’ number, size, and density distribution as well as their initial velocities. It is widely agreed that heavy droplets will deposit within less than a meter [3] while micron-size airborne pathogen droplets could travel to a much longer distance following the air background stream [4]. Nonetheless, the effectiveness of such physical distance policies is found to be controversial on many occasions as the bioaerosol release mechanism from respiration, sneeze, and coughs are chronically underestimated in past studies. The places of disagreement in contradictory findings associated with the disease transmission are in numerous strands, including carriage process of pathogens with droplets and aerosols from an infected person to a new host, drying and evaporation processes of exhaled bioaerosols in accordance with their properties (e.g., size, mucus), environmental conditions (e.g., relative humidity), and number and size of released bioaerosols in each activity mode.
(i.e., respiration, sneeze, and coughs). One should add the importance of demographical characteristics (age, gender, etc.) on the airborne pathogen droplets’ release mode as it has been broadly addressed in previous studies. Some of these understandings are summarized as 12 pivotal factors in Table 1.

### Table 1. List of effective factors in airborne pathogen droplets’ release.

| #  | Item [unit]           | Reported Interval             | Reference |
|----|----------------------|-------------------------------|-----------|
| 1  | Bioaerosol size distribution [μm] | 0.5 – 2,000                  | [5]       |
| 2  | Number of bioaerosol/particles | 5,000, 9×10^6                | [5]       |
| 3  | Environment property  | Walls, windows, etc.          | -         |
| 4  | Local ambient air velocity [m/s] | [0.25-1.5], 21.7, 0- 10        | [6]       |
| 5  | Local ambient air direction [deg] | -                           | [7]       |
| 6  | Local ambient air humidity [%]    | [20 – 60], 50                | [6]       |
| 7  | Local air temperature [°C]       | [17-23], 25,                | [6]       |
| 8  | Temporal profile of exhalation flow rate (for C or S) [m^3/s] | -                          | [8]       |
| 9  | Spatial profile of exhalation [·] | -                           | [9]       |
| 10 | With or without facial mask      | [with or without]            | [10]      |
| 11 | Gender [·]                     | Man, Woman                    | [11]      |
| 12 | Age [year]                     | 19 - 50                       | [12]      |

The identified parameters in Table 1 are fully/partially supported by experimental and observational studies from various methodological perspectives, including medicine, statistics, fluid dynamics, etc. Yet, the role of airflow transport as the delivery route of pathogens in smaller size droplets (< 50 µm) is not well investigated while larger size droplets (> 50 µm) are commonly accepted to follow ballistic trajectory mainly governed by gravity. More recently, the lingering of small-size airborne droplets (< 5 µm) is suggested to be another plausible root in airborne disease transmission [4]. Although advanced methods such as particle image velocimetry, shadowgraphy, and laser diffraction system for tracing particles have been around in-hand for years, these approaches were barely successful to extend the knowledge in tracing airborne disease transmission in buildings and built environment due to multiple reasons such as high expenses and time constraint of set up. In fact, in the case affording the cost and time, experimental studies only cover a limited spectrum of droplet size, number, injection velocities released from sources and face major limitations in monitoring smaller scale droplets.

Computational Fluid Dynamics (CFD) is therefore a cheaper alternative, which has been widely used to overcome the shortcomings of experimental and observational studies. In this respect, high-fidelity CFD models validated against observational datasets have been developed on Lagrangian perspectives as flexible tools to further investigate the parameters impacting the release and spreading of bioaerosols, in particular, being able to scrutinize the transport process of smaller scale droplets. Despite the necessity in the Lagrangian CFD models to trace the small particles, such models demand intensive computational resources, which hinder a comprehensive investigation over the airborne pathogen droplets’ release process in respect to its various affecting parameters. This intensive computational cost implies that these CFD models cannot directly represent a human as the source of release in many practical scenarios where multiple occupants interact in mechanically or naturally ventilated environments. Nonetheless, the development of a simplified, yet reliable, airborne pathogen droplet release model is vital to be employed in ventilation design and space management. In other words, unlike other well-investigated mass and heat transfer bio-sources sources such as CO₂ and heat rates, which are widely used for design and decision-making, airborne pathogen release rates from bio-sources are not well understood.

To address this shortcoming, this study aims to develop a simplified airborne pathogen spread model of sneeze and cough. This model encompasses a range of parameters related to the distribution of human sources and environmental conditions. A high-fidelity Eulerian-Lagrangian CFD setup is developed for simulation of a series of scenarios and to construct a dataset. Eventually, a simplified correlation model is developed over this dataset to predict the distribution of pathogen droplets in accordance with relative humidity and temperature of an environment in addition to the airflow rate of a respiratory event.

### 2. Method

#### 2.1. Airborne Pathogen Droplets’ Release

The holistic process of respiration, speech, sneeze, and cough (RSSC) can be modeled as a turbulent jet flow, which carries airborne pathogen droplets as illustrated in Figure 1. Within the turbulent jet,
droplets’ sizes significantly vary through their path line. While larger droplets (>50 µm) follow a ballistic trajectory, mainly governed by gravity, and therefore fall to the ground or settle on surfaces in a limited radius around their emitter, the intermediate droplets (10-100µm) and small droplets (<5 µm) are more affected by airflow and ventilation streams and may travel much further, especially after being dried. Quick evaporation makes the intermediate size droplets of RSSC to become airborne and stay floating in the air. For instance, the drying times for 50 and 100 µm droplets at 50% relative humidity are reported to be 0.3 and 1.3 s, respectively [13]. Even after complete evaporation, small airborne droplets can carry viruses as the usual size of viral pathogens is 25 nm to 5 µm and therefore a dried airborne may contain many of them. For the small droplets with low Stokes number (≪ 1), the sedimentation time is longer than the time needed for complete evaporation and the small droplets become airborne and, therefore, suspended in the air and move with the background airflow, increasing the risk of virus transmission to a much longer distance.

![Figure 1. Airborne pathogen airborne release mechanism in an enclosed environment](image1)

2.2. Proposed Framework of Airborne Pathogen Droplets’ Release Model

Comprehensive Eulerian-Lagrangian CFD modeling of airborne pathogen droplets’ release takes intensive computational cost even after using high-performance and cluster computing resources. Furthermore, the droplet release from bio-sources has been found to depend on several parameters as addressed in Table 1. This study proposes an innovative approach to substantially minimize the computational burdens while underpinning the necessary complexities of such phenomena. For this purpose, according to the framework shown in Figure 2, a high-resolution Eulerian CFD model (CFDe)
2.3. Eulerian CFD Model
The Eulerian method is applied to model the unsteady incompressible flow field using Navier-Stokes as the governing equations for mass, momentum, and energy equations:

\[
\frac{\partial u_i}{\partial x_j} = 0
\]  

(1)

\[
\frac{\partial u_i}{\partial t} + \frac{\partial (u_j u_i)}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left( \rho \frac{\partial u_i}{\partial x_j} - u_i' u_j' \right)
\]  

(2)

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_j} = 1 \frac{\partial}{\partial x_j} \left( k \frac{\partial u_i}{\partial x_j} + \left( \theta \frac{\partial u_i}{\partial x_j} - u_i' u_i' \right) U_j \right)
\]  

(3)

where \(u_i' u_j'\) is the Reynolds stress tensor, which is modeled by Boussinesq hypothesis. The SST k-\(\omega\) is also used as the turbulence model.

2.4. Lagrangian Discrete Phase Model
Particles are modeled based on a Lagrangian-Eulerian approach using Simcenter STAR-CCM+ where the conservation equations of mass, momentum, and energy for the dispersed phase are derived for each individual particle in a Lagrangian form to calculate their trajectories.

2.5. Equations of Motion for Particles
The trajectory of a discrete phase (i.e., particle, droplet, and bubble) is resolved by integrating a force conservation equation on each particle, written in a Lagrangian reference frame:

\[
\frac{du_i}{dt} = F_D(u - u_p) + g_i \frac{(\rho_p - \rho)}{\rho_p} + F_i
\]  

(4)

where “\(i\)” is the coordinate direction (\(i=x,y\) or \(z\)), and subscript “\(p\)” represents particles. \(u\) and \(\rho\) are the fluid phase velocity and density, respectively. \(F_i\) is the force per unit particle mass (acceleration), and the term \(F_D(u - u_p)\) represents an additional acceleration (force/unit particle mass) in which \(F_D\) is calculated as:

\[
F_D = \frac{18\mu}{\rho_p d_p^2} \frac{C_D Re}{24}
\]  

(5)

where \(\mu\) is the molecular viscosity of the fluid, and \(d_p\) is the particle diameter. Released bioaerosols from human sources are considered as discrete phases dispersed and carried out with airflow.

2.6. Particle Mass Balance
The equation related to the conservation of mass of a particle can be expressed as:

\[
\frac{dm_p}{dt} = m_p
\]  

(6)

where \(m_p\) denotes the mass of the particle, and \(m_p\) represents the rate of mass transfer to the particle. The latter is a non-zero value for the simulations, which include the evaporation process.

2.7. Droplet Evaporation
There are two common methods for the simulation of droplet evaporation, including quasi-steady single-component and multi-component droplet. The former assumes droplets to be composed of internally homogeneous single liquid such as a chemical species. The rate of change of droplet mass due to quasi-steady evaporation can be formulated as:

\[
\frac{dm_p}{dt} = m_p
\]  

(7)

where \(m_p\) denotes the mass of the particle, and \(m_p\) represents the rate of mass transfer to the particle. The latter is a non-zero value for the simulations, which include the evaporation process.
\[ m_p = -g^*A_s ln (1 + B) \]  
\[ (7) \]

where \( g^* \) represents the mass transfer conductance and \( B \) is known as the Spalding transfer number.

2.8. Particle Energy Balance

As a basic assumption for material particles, one can assume that particles are internally homogeneous. From a thermal point of view, this is equal to a low Biot number (< 0.1). The equation of conservation of energy will be:

\[ m_p c_p \frac{dx_p}{dt} = Q_t + Q_{rad} + Q_s \]  
\[ (8) \]

where \( Q_t \) is the rate of convective heat transfer to the particle from the continuous phase, \( Q_{rad} \) represents the rate of radiative heat transfer, and \( Q_s \) is related to other heat sources.

3. Case Study

After conducting a comprehensive literature review, three parameters, including droplet release velocity from bio-sources, room temperature, and room relative humidity are utilized as the effective parameters while considering a minimum three levels for each parameter. Each parameter is then varied with three and two increments to populate 27 and 18 scenarios for each respiratory event as presented in Table 2.

Table 2. Simulation scenarios.

| Respiratory Event | Parameter                  | Value         |
|-------------------|----------------------------|---------------|
| Cough             | Droplet release velocity   | 8m/s, 14m/s   |
|                   | Room temperature           | 15°C, 22°C, 29°C |
|                   | Room relative humidity     | 20%, 50%, 80% |
| Sneeze            | Droplet release velocity   | 18m/s, 34m/s, 50m/s |
|                   | Room temperature           | 15°C, 22°C, 29°C |
|                   | Room relative humidity     | 20%, 50%, 80% |

4. CFD Model Domain and Setup

The computational domain has a size of 3.5m × 3.5m × 6m as shown in Figure 3. Droplets produced by the exhalation, as presented in Table 3, were released from a circular area with a diameter of 1.2cm located at the center of a 3.5m × 3.5m wall. The dimensions of this domain have been selected after a series of preliminary simulations, ensuring the adequacy of the room dimensions for analysis of airborne behavior of the droplets where the exhalation jet reaches a velocity value in the order of 1cm/s. The simulations have been performed for different droplets with diameters from 0.1 to 100μm (see Table 3). The results implied that after simulating an adequate physical time, droplets with the diameter of 10μm or below linger in a range up to 6m from the releasing surface with a velocity below 0.02m/s while droplets with the diameter of 100μm are deposited in smaller distances of about 1m from the jet inlet.

Air is modeled as an ideal gas while the airflow is assumed to be isothermal, steady-state, turbulent, and incompressible. The double-precision pressure-based solver with the SIMPLE algorithm is used to model the velocity-pressure coupling. A convergence criterion was set as \( 10^{-5} \sim 10^{-6} \) for all conservation equations. All the employed boundary conditions are shown in Table 3.

Table 3. Boundary conditions of pathogen airborne CFD simulations.

| Boundary Type   | Boundary condition | Boundary Value |
|-----------------|--------------------|----------------|
| Inlet           | Velocity Inlet     | 8.3 m/s        |
| Outlet          | Outlet Pressure    | 1 bar          |
| exhalation jet temperature | Constant Temp. | 37°C           |
| Walls           | No slip            | -              |
| Droplet size and number | Figure 3 | Figure 3       |

As seen in Figure 4, the mesh was generated using hexahedral cells by Star CCM+. To capture small vortices and high velocity gradients near the jet entrance as well as alongside of the centerline of the
domain in both cases, both meshes have been refined at those places. On the surfaces, the final mesh has minimum size of 0.06m and maximum of 0.2m together with the surface growth rate of 2.0. This results in the blocks between 0.78mm near the mouth to 0.8m at the central part of the domain.

![Figure 3](image3.png)

**Figure 3.** Extracted velocity profile of (a) cough [6], and (b) sneeze [15] and droplet size histogram of (c) cough [16], and (d) sneeze [17]

![Figure 4](image4.png)

**Figure 4.** Mesh distribution around the jet centerline

![Figure 5](image5.png)

**Figure 5.** Comparing the centerline velocity of CFD with the experimental data presented in [14]

5. CFD Model Validation and Calibration

Prior to main simulations, a mesh sensitivity analysis (ranging from 189k to 4.5M cells) has been performed to reach an optimum mesh configuration, as shown **Figure 4**. For this part, the flow velocity in the far field zone (at a distance of \( y/d_0 > 20 \) from the mouth) has been investigated, and the
normalized results were compared with the experimental results as shown in Figure 5. For the validation scenario, the inlet velocity had spanwise as well as streamwise velocity profiles [14] with the maximum value of 8.3 m/s. It should be noted that in the case of validation there is no temperature difference throughout the domain. The results exhibit a good agreement between the simulations and the experimental results.

6. Results
At this stage, a risk index of the safe distance is developed where, at each point of the domain, the summation of the droplets passed during a specific period is calculated. A minimum of 100 droplets is reported as the minimum dosage of infection [18]. So, only the regions with higher than 100 accumulated particles are considered as a threshold of disease transmission proposed by [18]. Figure 6 illustrates the planar representation of the accumulated distribution of droplets injected via a cough with a velocity of 14 m/s in a room with a temperature of 14°C and relative humidity of 80% after 80 seconds. The risk index of the safe distance varies from 0.5 to nearly 1.8 m as exposure time rises from 10 to 80 seconds.

Considering the simulation parameters presented in Tables 2 and 3, the reliability of this method to predict the accumulative behavior of the droplets requires that it differentiates the spread patterns of various exhalation activities at the specified range of temperature and relative humidity levels. For this purpose, scenarios in Table 2 are simulated and analyzed using the explained method. The horizontal and vertical spread risk of these scenarios are then calculated and fitted to a linear regression model while the coefficients were obtained by applying as the below the least square equations method:

$$y_i = A_i x_1 + B_i x_2 + C_i x_3 + D_i$$

(9)

where $x_1$ is the injection velocity (m/s), $x_2$ is the room temperature (°C), $x_3$ is the room relative humidity (%), $y_1$ and $y_2$ are the horizontal and vertical spreads (m), respectively. The coefficients are provided in Table 4.

| Table 4. Coefficient of linear regression. |
|-------------------------------------------|
| Horizontal spread (y$_1$) | Vertical spread (y$_2$) |
|--------------------------|------------------------|
| A  | 0.0285 | -0.0047 |
| B  | 0.0024 | -0.0454 |
| C  | -0.0002 | -0.0081 |
| D  | 0.4888 | 3.0414 |

7. Conclusions and remarks
A new prediction method was developed to find the accumulative concentration of infectious exhaled droplets using a series of CFD simulations. Once the spread distances were calculated for multiple scenarios with the variation of the pathogen droplet release’ velocity, and rooms’ temperature and relative humidity, the data were fitted in a regression to develop a simplified model. Calculated results indicated that there was a meaningful difference between the spread patterns of selected cases (mainly related to the room temperature and relative humidity) which makes it a proper choice to investigate safe social distance evaluations under different conditions. This prediction method in addition to other
advanced methods (e.g., exponential, and neural network) can be also applied to re-link safe social distance according to exposure time to infectious sources.

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