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A simplified tempo-spatial model to predict airborne pathogen release risk in enclosed spaces: An Eulerian-Lagrangian CFD approach

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ABSTRACT

COVID19 pathogens are primarily transmitted via airborne respiratory droplets expelled from infected bio-sources. However, there is a lack of simplified accurate source models that can represent the airborne release to be utilized in the safe-social distancing measures and ventilation design of buildings.

Although computational fluid dynamics (CFD) can provide accurate models of airborne disease transmissions, they are computationally expensive. Thus, this study proposes an innovative framework that benefits from a series of relatively accurate CFD simulations to first generate a dataset of respiratory events and then to develop a simplified source model.

The dataset has been generated based on key clinical parameters (i.e., the velocity of droplet release) and environmental factors (i.e., room temperature and relative humidity) in the droplet release modes. An Eulerian CFD model is first validated against experimental data and then interlinked with a Lagrangian CFD model to simulate trajectory and evaporation of numerous droplets in various sizes (0.1 μm–700 μm). A risk assessment model previously developed by the authors is then applied to the simulation cases to identify the horizontal and vertical spread lengths (risk cloud) of viruses in each case within an exposure time. Eventually, an artificial neural network-based model is fitted to the spread lengths to develop the simplified predictive source model. The results identify three main regimes of risk clouds, which can be fairly predicted by the ANN model.

1. Introduction

The primary transmission mode of COVID19, as a rapidly spreading airborne disease, 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 worldwide while the essence of such stipulated measures is adapted from early evidence regarding the release and environmental persistence of SARS-CoV2 [2].

From fluid dynamics perspectives, COVID19 transmission mode via respiratory bioaerosols requires a thorough investigation of droplets’ number, size, and density distribution as well as their initial velocities [3]. It is widely agreed that heavy droplets will deposit within less than a meter [4] while micron-size droplets could travel to longer distances following the air stream [5]. Nonetheless, the effectiveness of such physical distance policies is controversial on many occasions as the bioaerosol release mechanisms from respiration, sneeze, and coughs are chronically underestimated in past studies. Respiration, speech, sneeze, and cough (RSSC) flows carry bioaerosols, the size of which significantly varies through the particles’ path line. Larger droplets (>50–100 μm) are commonly accepted to follow ballistic trajectories being mainly governed by gravity. The intermediate (10–100 μm) and small (<5–10 μm) droplets are more affected by airflow and ventilation streams and may travel much further. At the same time, the evaporation process changes the intermediate size droplets of RSSC to become airborne and stay floating in the air, which particularly highlights the role of

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ventilation and air humidity. For instance, the drying times for 50 μm and 100 μm droplets at a 50% relative humidity are reported to be 0.3 and 1.3s, respectively [36]. Even after a complete evaporation, small dried aerosol particles can potentially carry viruses as the usual size of viral pathogens is 25 nm to 5 μm [5]. For small droplets with a low Stokes number (St ≪ 1), the sedimentation time is longer than the time needed for a complete evaporation process, and the small droplets become airborne. Therefore, they turn suspended in the air and move with the air stream, increasing the risk of virus transmission to a much longer distance. More recently, it is suggested that lingering small size airborne droplets (<5 μm) can be a major plausible root in airborne disease transmission [21]. A schematic description of bioaerosol behaviour is shown in Fig. 1.

The place 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 [16], drying and evaporation processes of exhaled bioaerosols following with its properties (e.g., size, mucus), environmental conditions (e.g., relative humidity) [5-17], and number and size of released bioaerosols in each activity mode (i.e., respiration, sneeze, and coughs) [8,18,19]. As it has been broadly discussed in previous studies, one should add the importance of demographical characteristics (age, gender, ethnicity, etc.) on the bioaerosol release mode. Some of these understandings are summarized as 12 pivotal factors in Table 1. These are the effective parameters that may influence bioaerosol release and dispersion. Many of these parameters ultimately alter the volume and speed of respiratory droplets release and therefore can be represented by the velocity of a two-phase respiratory flow at the mouth. Hence, in this study, the effective parameters are shortlisted to three major ones to lower the computational costs and carry out the calculations in a practical timeline.

The identified parameters in Table 1 are supported by careful experimental and observational studies from various methodological perspectives, including medicine, statistics, fluid dynamics, etc. For example, the National Institute for Occupational Safety and Health [20] constructed a cough aerosol simulator that produces a humanlike cough in a controlled environment based on coughs recorded from influenza patients. The total aerosol volume expelled during each cough was monitored to be 68 μl using aerosol generated from a cell culture medium. As a PIV study to measure coughing velocity, Kwon et al. [12] obtained the average initial coughing velocity of 15.3 m/s for males and 10.6 m/s for females while the average initial speaking velocity was obtained the average initial coughing velocity of 15.3 m/s for males and 10.6 m/s for females while the average initial speaking velocity was 0.25–1.5 m/s, 21.7, 0-10 [7,8].

Table 1

| #   | Item [unit]     | Reported Interval       | Reference |
|-----|-----------------|-------------------------|-----------|
| 1   | Bioaerosol size distribution [μm] | 0.5-2,000 | [4,6]     |
| 2   | Number of bioaerosol/particles | 5,000, 9 × 10^6 | [6,7]     |
| 3   | Environment property | Walls, windows, partitions, etc. | [7]       |
| 4   | Local ambient air velocity [m/s] | [60-60], 20 | [6,8]     |
| 5   | Local ambient air humidity [%]  | 25-75 | [6,8]     |
| 6   | Local ambient air temperature [°C] | 17-23 | [7,8]     |
| 7   | Temporal profile of exhalation flow rate (for C or S) [m³/s] | 6,9 | [8,10,11] |
| 8   | Spatial profile of exhalation [°C] | 20 | [12,13]   |
| 9   | Utilization of facial mask [with or without] | [7,8] | [11]     |
| 10  | Gender [–]             | Man, Woman | [14]     |
| 11  | Age [year]             | 19-50 | [15]     |

32° for the females while that of the exhaled air from speaking was around 49° and 78°, respectively. In another clinical experiment, the size of droplets were measured in an indoor environment with an air temperature of 18 °C and relative humidity of 50%; the horizontal range of large respiratory droplets (diameter 120 μm–200 μm) in speaking were between 0.16 m and 0.68 m, in coughing, between 0.58 m and 1.09 m, and in sneezing between 1.34 m and 2.76 m [32]. Also, results from comparative studies on transport characteristics of contamination dispersion in a passengers’ local environments revealed significant increases of residence times (up to 50%) and extended travel distances of contaminants up to 200 μm after considering cough flow, whereas contaminants travel displacements still remained similar [33]. In a conditioned indoor environment, Zhang et al. [8] reported the distribution of generated aerosol from a horizontal coughing mode using a manikin in the presence of 16 diffusers mounted on walls. In another study, an experimental cough aerosol detection via laser diffraction system from 45 healthy people presented a demographic statistical analysis of bioaerosol sizes varying by sex and age [15]. Although advanced methods employed to obtain the mentioned results, including particle image velocimetry [22,23], and laser diffraction system [15] to trace particles, have been around in-hand for years, these approaches were barely successful in extending the knowledge in tracing airborne disease transmission in buildings and the built environment. The reasons are due to the high expenses, time constraint of set up, and limitation of devices in monitoring smaller scale droplets while experimental studies only cover a limited spectrum of droplet size, number, injection velocities released from sources (i.e., the mouth of people).
Computational Fluid Dynamics (CFD) is a cheaper alternative that widely being 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 [5], particularly the transport process of smaller scale droplets. For example, the movement of occupants in the room, due to its impact on airflow patterns inside the enclosed areas, was a subject of several CFD studies. Shih et al. [24] numerically investigated the impact of occupants’ movement as well as the door opening and closing on the flow distribution inside a hospital isolated room. They found that both movement and door sliding have temporal impacts on the flow distribution inside the investigated room.

In another study, Wang et al. [25] employed CFD to investigate the impact of walking on the dispersion of exhaled droplets in an isolated room. Their simulation results showed that the local environment around the occupant could be affected by walking. They also reported that increasing the walking speed decreases the concentration of suspended airborne particles. Some of the other numerical studies addressed the human respiration process and the transport of exhaled air by breathing, sneezing, and coughing, and their potential impact on the adjacent person [25–28]. Discrete and continuous models of droplets in multiphase turbulent buoyant clouds are studied by [29] with suspended droplets of various sizes. These studies highlighted that cough and sneeze airflows are multiphase turbulent buoyant clouds with suspended droplets of various sizes. The droplets can remain suspended in the cloud until their settling speed matches that of the decelerating cloud. In addition, the 3D transient CFD model is used by [30] to predict personal exposure times to airborne pathogens and thus the infection risk in a displacement ventilated room. Authors showed that for short separation distances, the interaction between breaths is a key factor in the airborne cross-infection. Li et al. [31] studied the evaporation and dispersion of cough droplets by a Lagrangian-Eulerian model in quiescent air, considering an inhomogeneous humidity field, and demonstrated that evaporation-generated vapor and super-saturated wet air exhaled from the respiratory tracks can form a vapor plume in front of the respiratory tract opening. Interestingly, due to the droplet size reduction induced by evaporation, both the numbers of airborne droplets’ density and mass concentration of inhalable pathogens remarkably increased, which may elevate the risk of infection.

In addition to these studies, the physics of droplet dispersion and distribution were investigated from mouth coughing and nose breathing using LES by [5,8]. It was reported that the typical size range of speech distribution were investigated from mouth coughing and nose breathing lets reduction induced by evaporation, both the numbers of airborne drop the respiratory tract opening. Interestingly, due to the droplet size exhaled from the respiratory tracks can form a vapor plume in front of demonstrated that evaporation-generated vapor and super-saturated wet air dispersion of cough droplets by a Lagrangian-Eulerian model in quies dispersion of cough droplets in a fever clinic showed that the best ventilation performance appears for a patient sitting and coughing while the case of a patient lying and talking was the worst case [31].

Despite the necessity to employ Lagrangian CFD models to trace the small particles, such models demand intensive computational resources, which hinder a comprehensive investigation of the bioaerosol release process regarding its various affecting parameters. This implies that Lagrangian simulations are costly choices to be directly applied to represent humans as the source of bioaerosol release in many practical scenarios where multiple occupants interact in mechanically or naturally ventilated environments. Nonetheless, developing a reliable bioaerosol release source is vital for the design and control of ventilation design, space management, and social distancing, especially during pandemics. Hence, similar to many other simplified source term models of a human body such as the amount of heat or CO2 releases widely used in buildings’ design and control applications, a simplified airborne pathogen droplet release model is necessary to be applied as a source term into other associated models.

To address this shortcoming in providing a deep insight related to virus-laden bioaerosol release from human sources in indoor and outdoor spaces, this study proposes a framework to develop a simplified model of droplets’ release from respiratory events (here sneeze and cough). This model encompasses a range of droplet release modes related to clinical (i.e., droplet release velocity from the bio-source mouth) and environmental (i.e., room temperature and relative humidity) distribution of bio-sources using an Eulerian-Lagrangian CFD model. The effective parameters on droplet release from bio-sources are initially synthesized to define a series of airborne pathogen release scenarios (35 cases). These scenarios are then simulated with a series of computationally intensive Eulerian-Lagrangian CFD simulations to construct a dataset for repository release droplets. The dataset is then fed into a risk assessment model (RAM) previously developed by authors [35] to account for the tempo-spatial risk analysis of the respiratory event rather than the instantaneous release of droplets. In a latter step, the tempo-spatial risk data is fitted to an artificial neural network (ANN) model capable of predicting the risk cloud expansion of a bio-source throughout time. It should be noted that the background airflow of the studied enclosed space is assumed as still air condition, so that the initial behavior of droplets’ transport can be observed. The human source is considered to have a fixed position in the room, and its movement is not taken into account in this study. Nonetheless, the proposed framework demonstrates the flexibility to add any complex background airflow that may be caused by bio-source movement, ventilation systems, etc.

In addition, to develop the artificial intelligence (AI) model to predict numerical results of CFD simulation, the multi perceptron feedforward ANN is adopted with deep learning to generate an accurate prediction for unseen conditions. The ANN code is developed in Python program language, and the number of neurons as well as other settings such as learning rate are tuned, and tailored for this specific work.

Regarding the structure of this paper, Section 2 describes the methods used to develop the Eulerian-Lagrangian CFD model risk assessment model. It also briefly explains the risk assessment model. Section 3 presents the scenarios designed to cover a range of airborne pathogen release modes. Finally, Section 4 provides the results, followed by the discussions and conclusion sections.

2. Method

2.1. Proposed framework of airborne pathogen respiratory aerosol release model

As stated before, comprehensive Eulerian and Lagrangian CFD modeling of airborne pathogen respiratory aerosol release takes intensive computational cost even after using high-performance and cluster computing resources. Furthermore, as addressed in Table 1, the bioaerosol release has been found to depend on several parameters. Thus, reaching a comprehensive model, undertaking airborne pathogen respiratory droplets release rate of any individual, is an impractical approach. Hence, this study proposes an innovative approach to substantially decrease the computational burdens while underpinning the necessary complexities of such phenomena. The proposed framework benefits from different tools to systematically develop a simplified model to be used for ventilation design or social distancing control in spaces.

For this purpose, as depicted in the framework of Fig. 2, four steps are considered to generate the simplified bio-source model. In Step-1, an Eulerian CFD model is first developed to accurately replicate the flow field in a room with a still background airflow field. While the buoyancy effect due to the room temperature stratification and jet release
temperature is taken into account, the flow streams are successfully validated with an experimental study by [39].

Step-2 is dedicated to accurately modeling large to small droplet movements via a Lagrangian CFD model, which is then coupled with the Eulerian model to reproduce the velocity field at an acceptable level while fast due to its low and yet precise enough number of cells. At this stage, parameters of Table 1 have been analyzed and shortlisted to the three most important ones (i.e., bio-source velocity, room temperature, and room RH). Thirty-five scenarios have been generated to cover a wide range of rooms’ conditions and bio-source release velocities related to sneeze and cough modes. It should be noted that due to the extensive range of rooms and room RH. Eventually, in Step-4, the calculated maximum distances (risk clouds) of all case studies generated in the previous step are used to train a simplified model using the artificial neural network technique. In this model, the release velocity, room temperature, and RH are the inputs, and the tempo-spatial risk cloud is the output.

2.2. Eulerian CFD model

An Eulerian method is applied to model the unsteady incompressible flow field using Navier-Stokes as the governing equations for mass, momentum, and energy equations:

\[
\frac{\partial U_i}{\partial t} + \frac{\partial (U_i U_j)}{\partial x_j} = - \frac{1}{\rho} \frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left( \underbrace{\frac{\partial U_i}{\partial x_j} - \overline{u_i u_j}}_{\text{viscous stress tensor}} \right) \tag{1}
\]

\[
\frac{\partial T}{\partial t} + \frac{\partial (U_i T)}{\partial x_i} = \frac{1}{\rho C_p} \frac{\partial}{\partial x_i} \left( k \frac{\partial T}{\partial x_i} - \overline{u_i u_j} U_j \right) \tag{2}
\]

where \(\overline{u_i u_j}\) is the Reynolds stress tensor, which is modeled by the Boussinesq hypothesis.

2.3. Lagrangian discrete phase model

Particles are modeled based on a Lagrangian-Eulerian approach using SimcenterSTAR-CCM + Ver. 13.06.12 (double precision), where the conservation equations of mass, momentum, and energy for the dispersed phase are derived for each particle in a Lagrangian form to calculate their trajectories.

2.3.1. Equations of motion for particles

As a general method for particles, droplets, and bubbles, the trajectories of discrete phases (i.e., respiratory droplets) are resolved by integrating a force conservation equation on each particle, written in a Lagrangian reference frame:

\[
\frac{d u_p}{dt} = F_D (u - u_p) + g (\rho_p - \rho) \tag{4}
\]

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. \(F_D\) is the force per unit particle mass (acceleration), and the term \(F_D (u - u_p)\) represents an additional acceleration (force per unit particle mass) in which \(F_D\) is calculated as:

\[
F_D = \frac{18 \mu c_D Re}{\rho_p d_p^2 / 24} \tag{5}
\]

where \(\mu\) is the molecular viscosity of the fluid, and \(d_p\) is the particle diameter. Also, \(Re\) is the relative Reynolds number, which is calculated as:

\[
Re = \frac{\rho (u - u_p) d_p}{\mu} \tag{6}
\]

Since the dispersed droplets are volatile, a mass transfer occurs between the phases accompanied by an interphase heat transfer. Hence, a heat transfer occurs because of the interphase temperature differences while the interphase mass transfer changes the sizes of the droplets as described in the following sub-sections.

2.3.2. Particle mass balance

The equation related to the conservation of mass of a particle can be expressed as:

\[
\frac{d m_p}{dt} = \dot{m}_p \tag{7}
\]

where \(m_p\) denotes the mass of the particle, and \(\dot{m}_p\) represents the rate of mass transfer to the particle. The latter is a non-zero value for the simulations, which includes the evaporation process.
2.3.3. Droplet evaporation

The multi-component droplet evaporation model used in this study assumes droplets to be internally homogeneous, consisting of an ideal mixture of liquid components subject to vaporization. Moreover, the model assumes inert components in both the droplet and the gas. Regarding the evaporation of multi-component droplets, \( m_{pe} \) is defined as the rate of change of mass of each transferred component due to a quasi-steady evaporation:

\[
m_{pi} = - \varepsilon_i g^* A_i \ln(1 + B) \tag{8}
\]

where \( g^* \) represents the mass transfer conductance, and \( B \) is known as the Spalding transfer number. Also, \( \varepsilon_i \) is the index of each component in the mixture, and \( \varepsilon_i \) represents the fractional mass transfer rate for which the sum of all \( N \) components complies with the following equation:

\[
\sum_{i=1}^{N} \varepsilon_i = 1.0 \tag{9}
\]

2.3.4. 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 can be expressed as:

\[
m_{pi} c_i \frac{dT_i}{dt} = \dot{Q}_i + \dot{Q}_{rad} + \dot{Q}_s. \tag{10}
\]

where \( \dot{Q}_i \) is the rate of the convective heat transfer to the droplets from the continuous phase, \( \dot{Q}_{rad} \) represents the rate of the radiative heat transfer to the droplets from other particles, and \( \dot{Q}_s \) is related to other heat sources.

2.4. CFD domain, mesh, and boundary conditions

The computational domain has a size of 3.5 m × 3.5 m × 6 m as shown in Fig. 3, representing a room without ventilation. Droplets with different diameters from 0.1 μm to 700 μm, caused by the exhalation, were released from a circular area with a diameter of 1.2 cm located at the center of a 3.5 m × 3.5 m wall [30]. It is worth noting that the mouth diameter (1.2 cm) has been chosen slightly smaller than the value of 1.5 cm that was used by Chao et al. [44] for the average mouth diameter of eight university students (under 30 years old). While these two values are in the same range, the smaller mouth diameter in the present research assumes that the respiratory event might be released by patients of younger ages or smaller body sizes.

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 2 cm/s (less than 1% of the jet velocity) before it reaches the wall in the front of the side of the mouth (located at \( x = 6 \) m) [41]. The results implied that after simulating an adequate physical time, droplets with the diameter of 10 μm or below linger in a range up to 6 m from the releasing surface with a velocity below 2 cm/s while droplets with the diameter of 100 μm are deposited in the smaller distances of about 1 m from the jet inlet.

To ensure the final size of the utilized mesh being in a reasonable range, different grid resolutions with hexahedral cells were tested, ranging from 189 k cells to 4.5 M cells. The optimal mesh was identified as the 189 k-HYB case, which has minimum and maximum cell sizes of 0.06 m and 0.2 m, respectively, with a surface growth rate of 2.0. It should be noted that a conic volume with a length of 1 m dense cells was generated around the mouth of the bio-source as seen in Fig. 3. All surfaces were considered as solid walls with no-slip boundary conditions. The other boundary conditions of the model are presented in Table 2.

A proper simulation of an exhalation activity requires reliable data on the size distribution of droplets in addition to a reliable transient exhaled airflow profile. Fig. 4 presents the air velocity profiles and droplet size distributions of sneeze and cough, resulting from measurements conducted on numerous people of different ages and gender.

### Table 2

Droplet and background air properties.

| Droplet properties | Mass fraction [%] | Density [kg/m³] | Specific heat capacity [J/(Kg•K)] | Saturation pressure [Pa] |
|--------------------|-------------------|-----------------|-----------------------------------|--------------------------|
| Non-evaporative Air Properties | Dynamic viscosity [Pa-s] | Molecular weight [Kg/ Kmol] | Specific heat capacity [J/(Kg•K)] | Saturation pressure [Pa] |
| 3 [42] | 1,003.6 | 1,280.8 | 2,404.6 |
| 97 [43] | 997.6 | 1,855 × 10⁻⁵ | 28.97 | 1,003.6 |
| 4,181.7 | 3,170.3 |
| 4,181.7 | 3,170.3 |

Profiles in Fig. 4

![Fig. 3. Mesh distribution around the jet centerline.](image-url)

\[\text{Fig. 3. Mesh distribution around the jet centerline.}\]
2.5. CFD setting

In the present transient CFD simulations, the background air was simulated as a non-reactive ideal gas composed of standard air and some amount of water vapor, depending on the relative humidity of each case (see Table 2). The results of the simulations, conducted within 60 s, implied that the droplets with a diameter of 10 μm or below had become airborne, traveling not more than 5 m from the mouth, while droplets with a diameter of 100 μm fell at short distances of about 1 m from the jet inlet.

The droplets were simulated as discrete phases using the Lagrangian model and were assumed to have spherical shapes. To mimic realistic pathogenic droplets, they were assumed to be initially composed of 3% non-evaporative and 97% evaporative mass fractions. The density of the non-volatile fraction was 1,280.8 kg m$^{-3}$ with a specific heat transfer of 2,404.6 J Kg$^{-1}$K$^{-1}$ at the standard state temperature of 298.15 K. On the contrary, the evaporative portion was assumed as water with a density of 997.6 kg m$^{-3}$ and a specific heat transfer of 4,181.7 J Kg$^{-1}$K$^{-1}$ at the same standard state temperature. In addition, the saturation pressure of this evaporative fraction (water) was set to 3,170.3 Pa. The mass-weighted mixture was used for the calculation of the density and specific heat of each droplet. Furthermore, it was assumed that the droplets would stick to any wall surface of the room as they reached to. As an averaged value, the time span of cough and sneeze were considered 0.6 s. At each simulation, after the cough or sneeze periods, the droplets’ release were modeled by a sinusoid breathing with the maximum velocity of about 1 m/s and intermittence of 5 times for one minute.

Similar to the Lagrangian model, the weighted mixture method for the Eulerian model was employed for the calculation of the air-water mixture in the background air. Finally, the aerodynamic interaction between the particles and the air has been simulated using drag force calculated by Schiller–Naumann’s drag force coefficients and the pressure gradient force.

The turbulence was modeled using Realizable k-epsilon model with “All y+ wall treatment” option in STARCCM, making the model suitable for the coarse and fine meshes. It should be noted that the Realizable k-epsilon is classified under High Reynolds Number turbulence models, and its y+ can be 100 or even higher. In the present simulations, the y+ was about 10, which is out of the critical range [11.04–30]. In addition, the “two-layer, all y+ wall treatment” option in STARCCM adjusts the wall functions for any y+ in areas near the mouth with smaller y+ [40].
It is also worth mentioning that since the present model does not work with any flow details near the walls, the flow velocity near the walls was almost zero.

The discretization method was selected as a second-order scheme for the momentum equations. The energy equation was activated to include the evaporation of the droplets. All simulations were conducted as transient simulations with a timestep of 0.01 s with 20 inner iterations. Due to the high computational cost of the transient solution, the level of convergence was set not smaller than $10^{-4}$. Yet, each case was taken about 16 h for a typical simulation time for 60 [s] using the computer cluster at Sogang University with 24 computational cores with Xeon(R) 2.20 GHz CPUs.

2.6. Risk assessment model

When performing Lagrangian simulations, CFD solvers mainly report instantaneous data of droplets such as position, velocity, and diameter. Nonetheless, the infection risk at each position of the room is associated with the accumulated number of droplets passing from that point within a specific time interval. On the other hand, medical evidences suggest that a disease transmission with airborne pathogens happens when a person inhales a certain dosage of infected droplets.

A previously developed risk assessment model (RAM) by authors thus calculates the accumulated droplets passing at each space location. For this purpose, RAM generates a uniform coarse mesh inside the domain, known as the secondary mesh (shown in Fig. 5). In accordance to available output data of droplets generated by the CFD solver at each time-step, the secondary mesh predicts the position of droplets at previous time-steps and consequently computes the accumulated number of droplets at each cell of the secondary mesh within the time-span of the simulation. RAM includes multiple steps to count the number of droplets with different droplet sizes from sub-micron to hundreds-micron released from respiratory jet and passing through a specific location of an enclosed space. Therefore, this leads to a 3D temporal profile, which shows a temporal risk cloud being expanded around a bio-source. Details of RAM developed by authors and applied algorithm can be found in [34].

2.7. Artificial neural network

A deep ANN with feed-forward multi-layer perceptron architecture has been used in this study [46]. A back-propagation learning paradigm was employed to build the simplified model. The continuous nonlinear sigmoid function with smooth gradient was employed in the model due to its proven capability in making clear distinctions on predictions. A comparison was conducted among five different architecture of ANN in terms of hidden layers and number of neurons to find the best architecture that delivers the best predictive results. The analysis was performed under the circumstances that the ANN was fully unsighted on all 60 values (secondly-basis CFD data for 1 min) within each two test cases. As shown in Table 3, the $10 \times 10$ ANN was eventually selected due to showing the least averaged testing error among other architectures. More hidden layers can potentially result in overfitting due to the nature and size of the data.

3. Case study

3.1. Airborne pathogen release scenarios

Eulerian-Lagrangian CFD simulations were computationally cumbersome tasks to be conducted for many scenarios related to various airborne pathogen droplet releases from human sources. However, by implementing the design of experiment (DoE) technique, the intensive computational burden related to the number of required simulations was substantially reduced in this study. For this purpose, 12 parameters (e.g., droplet size, number of droplets, the temporal, and spatial profile of cough) were initially identified as the effective parameters (see Table 1). After scrutinizing a comprehensive literature review and

| NN Architecture | Averaged ANN training error | Averaged ANN testing error |
|-----------------|-----------------------------|---------------------------|
| $5 \times 5$ ANN | 13.3%                       | 34.2%                     |
| $9 \times 9$ ANN | 11.5%                       | 31.6%                     |
| $10 \times 10$ ANN | 9.25%                      | 29.6%                     |
| $20 \times 20$ ANN | 10.12%                     | 32.1%                     |
| $30 \times 30$ ANN | 12.9%                       | 33.7%                     |
implementing further assumptions when data do not exist, three parameters, including droplet release velocity from bio-sources, room temperature, and room relative humidity, were utilized as the effective parameters while considering a minimum of three levels for each parameter. Each parameter was then varied with three increments to initially populate 27 cases as presented in Table 4. After analyzing the data as presented in the results section, eight additional cases were added to improve the training of the ANN model. As mentioned in Section 2.7, each case has an array of 60 values on a secondly-basis that shows the evolution of the vertical spread over 60 s. Furthermore, two cases were used only to validate the model and were not included in the training steps. Although considering 35 cases is not ideal for three main identified parameters, the ANN results shown in the following sections reveal the capability of the model to capture a relatively correct vertical and horizontal spread, which satisfies the main aim of this study to develop a simplified model in recognizing such distances.

4. Results and discussion

4.1. Mesh sensitivity analysis

Since the most crucial parameter in droplets’ dispersion is the air velocity, before the main simulations, a mesh sensitivity analysis has been performed to ensure that the final mesh and velocity field are independent of the element size. For this purpose, the flow velocity in the far-field zone (i.e., the distance where \( y/d_0 > 20 \) from the mouth) is investigated, and the results are validated against the experimental by [39]. The inlet velocity has spanwise (along with the discharge hole radii) as well as streamwise (centreline) velocity profiles with the maximum value of 20 m/s. At this stage, four meshes with different resolutions with hexahedral cells are generated, containing a total mesh number of 189 k, 627 k, 3.7 M, and 4.5 M.

After this preliminary study, it is observed that a minimum number of 3.7 M cells is required for an independent mesh resolution. However, since this research requires a large number of simulations that could result in an unaffordable computational cost, and also aligned with the aim of this study to develop a simplified model, the viable solution is to generate a mesh, which is relatively fast and also provides results with a fair level of accuracy. Hence, after several attempts, a new mesh arrangement of 189k-HYB with a zonal improvement just before the mouth location is generated that could accurately follow the result of the models with 3.7 M and 4.5 M cells (Fig. 6). This optimal mesh, 189k-HYB case, has minimum and maximum cell sizes of 0.06 and 0.2 m, respectively, while its surface growth rate is 2.0. This results in a dense mesh within 0.8 m from the mouth at the central part of the domain. Table 5 summarizes the applied boundary conditions for the validation test.

4.2. Validation of Eulerian CFD model

The first step in the framework of Fig. 2 is to validate the CFD model. For this purpose, an experimental study by [39] was used for the validation process due to its resemblance to the CFD model. Due to the lack of reliable experimental data on buoyant air jets in the literature, the validation case used in this research work represents an isothermal non-buoyant jet, which helped validating the numerical setup applied to the continuum phase (air). The isothermal free turbulent jet experiment provides the spanwise and streamwise velocity profiles at its inlet location with a maximum value of 8.3 m/s. As expected, the Eulerian CFD model of the background flow is in a fair agreement with the experimental results reported by [39] as demonstrated in Fig. 6 while the air velocity at the centerline from the nozzle entrance (y = 0) up to the downstream distance of \( y = 50 d_0 \) is compared. Since the risk assessment model is more informative in far distances from the bio-source, it can be concluded that for such distances from the jet source \((y/d_0) > 10\), in general, the results are in a better agreement when are compared to the experimental data. As mentioned before, poor error observed at \((y/d_0) < 10\) regions was successfully resolved using a coarse mesh, but carefully adjusted size at different regions of the domain (189k-HYB). As a result, the maximum error observed at \((y/d_0) > 10\) region increases from 7% to 10% as it is switched from 4.5 M cell mesh to 189k-HYB. Thus, this mesh size considerably reduces CPU time from order of months to order of weeks where performing numerous numerical simulations were needed. The validation study with more details using multiple metrics can be found in [34].

Another similar set of experimental data reported by [47] is depicted

| Table 4 | Respiratory cough and sneeze simulation scenarios. |
|---------|---------------------------------------------------|
| Main cases | Case ID | Max. Velocity (m/s) | Room Temp. (°C) | Room RH (%) |
| 1, 2, 3 | 18 | 15 | 20, 50, 80 |
| 4, 5, 6 | 22 | 20, 50, 80 |
| 7, 8, 9 | 29 | 20, 50, 80 |
| 10, 11, 12 | 15 | 20, 50, 80 |
| 13, 14, 15 | 22 | 20, 50, 80 |
| 16, 17, 18 | 29 | 20, 50, 80 |
| 19, 20, 21 | 50 | 15 | 20, 50, 80 |
| 22, 23, 24 | 22 | 20, 50, 80 |
| 25, 26, 27 | 29 | 20, 50, 80 |

| Additional cases | Case ID | Max. Velocity (m/s) | Room Temp. (°C) | Room RH (%) |
| 28 | 34 | 29 | 60 |
| 29 | 34 | 15 | 10 |
| 30 | 25 | 25 | 65 |
| 31 | 18 | 18.5 | 50 |
| 32 | 34 | 29 | 70 |
| 33 | 34 | 29 | 75 |
| 34 | 25 | 15 | 50 |
| 35 | 25 | 15 | 20 |

| Validation (test) cases | T1 | 50 | 22 | 80 |
| T2 | 34 | 18.5 | 50 |

Fig. 6. Centreline velocity of CFD model compared to the experimental results by [39,47].
in Fig. 6 to better evaluate the numerical simulation. It should be noted that the maximum velocity of the recently mentioned research work is 56.2 m/s. Although numerical simulations show a higher deviation compared with experimental data of [47], the trend is still satisfactory with a smaller decrease in the downstream \((y/d_0) > 30\).

4.3. RAM model

The third step of the proposed framework is investigated in this section. As introduced in Table 4, 35 scenarios were simulated in this study, covering a wide range of respiratory droplet release events. As explained earlier, the RAM model [34] syntheses the CFD output data to generate an accumulative temporal status of droplets in front of a bio-source. The model counts droplets of any size at any location around the bio-source within the simulation time frame and marks that as a risky location when the number exceeds a defined critical threshold. Here, this value is defined as 100 following a study by [48]. Nonetheless, the model can be promptly adjusted to any other suggested numbers.

RAM is an effective tool to monitor the risk cloud expansion through time in a specific environmental and background flow condition. As seen in a base case of Fig. 7a, the vertical and horizontal spread of the risk cloud are separately illustrated after 1 min of droplets’ release of cough while the tendency of the risk cloud expansion is toward the ceiling. While the relative humidity of 20% is an extreme condition in a typical room temperature of 22°C, such information is handy to decide on the environmental control, HVAC design, and social distancing standards. This implies any person who stays 1 min in the 1.0 m vicinity of the bio-source can be subject to an infection. As shown in the following figure, time is a key in the airborne pathogen transmission, and while it is well understood, it is neglected in many risk-assessment studies.

When two out of three of the selected parameters are varied, as depicted in Fig. 7b–d, the risk cloud can drastically change. An example is Fig. 7b where a sneeze event is shown in an RH of 80%. Once again, a person should not stay in a 1.9 m vicinity of an infected bio-source for more than 1 minute. As shown in Fig. 7c, a sneeze in a hot and dry climate can even cause a stronger risk cloud both horizontally and vertically. Inversely, as initially suggested by many studies [49,50], a humid climate (e.g., RH > 60%) can yet be a safer environment in terms of disease transmission via airborne means. This marginal pattern of risk cloud expansion can be seen in Fig. 7d consistent with the former studies. The following sections will present the time evolution of these clouds in more detail.

In order to demonstrate the effects of ambient relative humidity on the variations of the plume and the movement of the droplets, the velocity fields and particle dispersions of cases 4 and 15 are shown in Fig. 8. Both cases have an identical temperature while the relative humidity and the sneeze velocity are different.

### Table 5
The boundary conditions of the validation case.

| Boundary Type | Boundary Condition | Boundary Value | Air Density | Air Dynamic Viscosity |
|---------------|--------------------|----------------|-------------|-----------------------|
| Inlet         | Velocity inlet     | 20 m s⁻¹       | 1.184 kg m⁻³ | 1.855 × 10⁻⁵ Pa s |
| Outlet        | Outlet pressure    | 1 bar          | -           | -                     |
| Walls         | No-slip            | -              | -           | -                     |

P.A. Mirzaei et al.

Building and Environment 207 (2022) 108428

Fig. 7. RAM model performance for a wide range of parameter variations; (a) Case 4, (b) Case 15, (c) Case 25, and (d) Case 9 after 60 s.
locations of the fallen heavier droplets depend on the sneeze velocity (the initial velocity of the droplets). However, since the locations of the airborne droplets are relatively the same, one can conclude that the transmission of these droplets is mainly affected by the relative humidity rather than the initial velocity. This finding can be explained by considering the fact that the small droplets lose their initial momentum because of the drag force, and then cannot travel very dissimilar from each other as the large droplets can. Since the initial sneeze velocity for these two cases are different, the small airborne droplets will follow different velocity fields created by two sneezes, leading to two different droplet dispersions.

In Fig. 9, a cough case study with a typical room temperature of 22°C
and a low RH of 20% is demonstrated for time snapshots of 10s, 20s, 40s, and 60s. While the risk cloud reaches 1.0 m only in few seconds, it is mainly vertically expanded from few centimeters to about the ceiling height. For this specific case, and as an example where extractors are ceiling mounted, RAM can help to attain similar environmental conditions in this room. Inversely, Fig. 10 shows a sneeze case (Case 27) with a temperature of 29°C and a high RH of 80% where the risk cloud is quickly expanded toward the ground and almost remains temporally invariant. Therefore, if a room has a ventilation system with a floor-mounted extractor, controlling the environmental condition toward achieving the same risk cloud expansion can be a better solution while enacting a 2.4 m distance rule between occupants.

4.4. Predictive model

The synthesized vertical and horizontal spread of RAM profiles of data cases in Table 4 is depicted in Fig. 11. As stated before, thirty-five training cases are simulated with the CFD model in addition to two testing cases.

Regarding the horizontal spread of the exhaled droplets for these 35 different conditions, as depicted in Fig. 11a, many of the curves are overlapped and cannot be distinguished from each other. Consequently, until t = 30 s, all cases can be classified into six groups in which no horizontal progress can be observed. It should be mentioned that in the horizontal risk measurement, the distance between two successive horizontal planes is 0.1 m. From the beginning of the numerical experiment (t = 1s), the horizontal spread of droplets starts at minimum values of 1 m for V = 18 m/s. As the exhalation velocity increases, the initial horizontal spread also increases such that for V = 50 m/s, the horizontal spread at the initial time-step reaches 1.8 m. In most cases, no evolution of the risk cloud on the horizontal spread is detected, mainly because of the particle dynamics due to drag and buoyant forces that progressively become significant in the vertical direction and change droplets to the upward direction.

Regarding the vertical expansion as illustrated in Fig. 11b, three main regimes can be identified in the data as highlighted in the graph. Regime I is associated with a sudden vertical expansion of the risk cloud (below 30s) when small droplets are affected by the buoyant plume of the exhaled jet. It should be noted that depicted lines represent the vertical spread of droplets, which does not necessarily reflect the air stream pathways. The upward motion of droplets is caused by the lifting up carrier phase and buoyancy, which is caused by the temperature difference between the exhaled flow and room temperature. An example is a cold and dry climate of Case 19 (temperature of 15°C and RH of 20%), where the jet plume is expected to push many of the droplets upward, undergoing quick evaporations while being broken to smaller droplets. Nonetheless, it should be mentioned that it is not a straightforward procedure to draw a general conclusion on the expansion pattern of the cloud risk. This further justifies the necessity of developing models similar to RAM to predict safe distances in complex environmental conditions. Regime II is a more frequent pattern for the risk cloud movement as droplets tend to gradually elevate toward the
ceiling. The pattern is again very complex to be generalized. Eventually, Regime III states those few cases mainly with a temperature of 29°C and RH of 80% (e.g., 9, 18, 27). The rate of evaporation in these cases is very low, and the plume is not very strong due to a lower temperature difference between the jet and room. Hence, a horizontal spread of the risk cloud can be seen in Fig. 11a.

Eventually, two samples from Regimes I and II are selected to show the performance of the training process after 1 M iterations using the backpropagation method. Regime III was omitted as its behavior is clearer to be predicted without using a complex predictive model. As mentioned before, the ANN inputs are velocity, temperature, humidity, and time where the output of the ANN is the spread of droplets in the vertical or horizontal directions. Also, the criteria to stop the training iteration of ANN is the discrepancy of the predicted value with respect to the CFD value to reach below a small value, namely 0.001. Moreover, it should be mentioned that the below-chosen test cases are considered as extreme prediction cases in which ANN did not priory include any of the temporal vertical spread evolution.

As seen in Fig. 12a, the expected values are plotted against ANN predicted values in addition to the lines of ±10% error. Fig. 12b shows the transient evolution of the vertical risk cloud predicted by the ANN model. The relative error of all test cases calculated by averaging 60 data samples in each training case is about 9.2% (i.e., 2,100 training data samples), which can be considered a fair relative error over the used datasets. Some cases in Regime I demonstrate higher relative errors (e.g., Case 24 with 14.2% error) due to the sudden change in the data pattern as the role of both buoyant and drag forces are simultaneously significant and challenging to be projected.

Fig. 10. Temporal performance of RAM model for Case 27 (Velocity = 50 m/s, Temp. = 29 °C, and RH = 80%).
effect on the averaged ANN training error is depicted in Table 6. For each step when the number of cases is increased, it is possible to evaluate the ANN training error. As the population of the training cases grows, the overall performance of the employed ANN increases while there is a decrease in the average and maximum values of the relative error for all cases.

5. Conclusion

Safe distance against airborne pathogen transmission is a parameter of space and the exposure time to various sizes of virus-laden droplets released from a bio-source. This paper proposes a framework to develop a simplified model to be assigned to bio-sources instead of running intensive CFD simulations to predict risk clouds released from them. A CFD model is first developed to simulate a range of parameters, covering many aspects of respiratory events, including clinical factors such as droplet release velocity, number and distribution of droplets, evaporation of droplets, and environmental factors, including room temperature and humidity. Then, 35 case studies have been defined and simulated to generate a comprehensive dataset. The CFD results have been analyzed based on a tempo-spatial risk assessment model [35] previously developed by the authors, which determines the vertical and horizontal
spread of respiratory droplets. An artificial neural network is then fitted to data to successfully predict the size of the risk cloud around a bio-source under different climatic and clinical conditions. According to the simulated cases, the vertical spread of droplets can be divided into three regimes with different trends. Some cases are under strong impact of plume while others are mildly or not influenced. Identification of such regimes is beneficial since they provide generalization in the behavior of the exhaled jets. It is also expected that the trained ANN to also reflect such generalization in its predictions. The results suggest that it is possible to apply ANN to a series of simplified CFD cases to generate a simplified calculation model for estimating safe social distances and ventilation designs under different environmental situations, which is more practical for non-experts to use.

Although the predicted results calculated by ANN are satisfactory for the test cases, successful implementation of the ANN tool to real cases needs more comprehensive CFD models that include background airflow, movement of subjects, a higher number of case studies, and also precise clinical data on the infective dosages. Hence, this study is an early step toward developing simplified models, and thus the developed CFD and RAM models can be subject to continuous improvements from the viewpoint of accuracy.

Future works should include other parameters such as background airflow impacted by occupants and ventilation means (mechanical and natural). Also, more simulations can be undertaken to enhance the performance of the predictive model. Eventually, more clinical data

![Fig. 12. (a) Training performance of ANN for the actual versus predicted values, and (b) the comparison of ANN model with the CFD simulation for Case 34 (Velocity = 25 m/s, Temp. = 15 °C, and RH = 50%).](image1)

![Fig. 13. ANN performance in prediction of (a) Case T1 and (b) Case T2.](image2)

| Table 6 | ANN relative error for different number of training cases. |
|---------|----------------------------------------------------------|
| Number of Training Cases | Averaged Relative Error | Maximum Relative Error |
| 5       | 27.9% | 59.4% |
| 15      | 18.3% | 45.8% |
| 25      | 13.7% | 31.5% |
| 35      | 9.2%  | 26.7% |
shall be collected to enhance the quality of the CFD model.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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