# CFD STUDY ON THE ADVECTION OF PARTICLE SIZE DISTRIBUTION OF DROPLETS \& AEROSOLS EXPELLED BY A TURBULENT JET 

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# CFD STUDY ON THE ADVECTION OF PARTICLE SIZE DISTRIBUTION OF DROPLETS \& AEROSOLS EXPELLED BY A TURBULENT JET 

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# ABSTRACT <br> CFD STUDY ON THE ADVECTION OF PARTICLE SIZE DISTRIBUTION OF DROPLET/AEROSOL PARTICLES EXPELLED BY A TURBULENT JET 

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Keywords: CFD, Particle Size Distribution, 2D Axisymmetric, Particle Tracking

In this research, study on the advection of particle size distribution was carried out using the 2D axisymmetric CFD model available in COMSOL Multiphysics v5.6. The aim of this research is gain insight into the movement of particles using a simplified 2D axisymmetric CFD model. The simplicity of the model allows for the relatively rapid generation of results as compared to the result generation time of high-fidelity 3D models and easy customization as opposed to experimental setups. The results presented here are focused on the change in the size distribution of particles that reach a target location and the fraction of the total particle volume initially emitted by the transmitter that reach a target location. Analysis of the results from different perspectives provide insight into the advective behaviour of the particles and the evolution of size distribution as the particles are delivered to target locations. To obtain the results, field flow simulations are carried out first, followed by particle tracking simulations.

## ÖZET

# TÜRBÜLANSLI BİR JET TARAFINDAN DIŞARI ATILAN DAMLACIK/AEROSOL PARTİKÜLLERİNİN BÜYÜKLÜK DAĞILIMININ ÖNERİLMESİ ÜZERİNE HESAPLAMALI AKIŞKANLAR DİNAMİĞİ ÇALIŞMASI 

# FIYINFOLUWA OLUWATOYOSI ABIOYE 

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Anahtar Kelimeler: Hesaplamalı Akışkanlar Dinamiği, Parçacık Büyüklüğü Dağılımı, 2 Boyutlu Eksenimetrik, Parçacık Takibi

Bu çalışmada, COMSOL Multiphysics v5.6'da bulunan 2 boyutlu eksenimetrik CFD (Hesaplamalı Akışkanlar Dinamiği) modeli kullanılarak partikül büyüklüğü dağılımının önerilmesi üzerine çalışma yapılmıştır. Bu araştırmanın amacı, basitleştirilmiş bir 2 boyutlu eksenimetrik CFD modeli kullanarak parçacıkların hareketi hakkında fikir edinmektir. Modelin sadeliği, yüksek doğruluktaki 3 boyutlu modellerin sonuç üretme süresine kıyasla nispeten hızlı sonuç üretilmesine ve deneysel kurulumların aksine kolay özelleştirmeye olanak tanır. Bu tezde sunulan sonuçlar hedef konuma ulaşan parçacıklar için sırasıyla parçacıkların boyut dağılımındaki değişime ve verici tarafından başlangıçta yayılan toplam parçacık hacminin oranına odaklanmıştır. Elde edilen sonuçların farklı açılardan analizi, parçacıkların adveksiyon (yatay iletim) davranışı ve boyut dağılımının evrimi hakkında fikir vermektedir. Bulunan sonuçları elde etmek için önce alan akış simülasyonları, ardından parçacık izleme simülasyonları gerçekleştirilir.

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I would like to thank Dr. Serhat Yeşilyurt for his consistent and dedicated support and guidance throughout the duration of this research.

Dedication page
I dedicate this thesis to my parents and siblings, whose unconditional love gave me the push I needed to stay focused and put in my best effort

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## 1. INTRODUCTION

### 1.1 Background

The emergence and outbreak of the coronavirus disease 2019 (COVID-19) began in December 2019. COVID-19 is a highly contagious disease caused by the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). Outlined in the World Health Organization (WHO) monthly situational reports and weekly epidemiological updates on COVID-19 (WHO, 2022), as of 16 January 2020, there have been a total of $21,294,845$ global reported cases and 761,779 global reported deaths. As of 17 July 2020, there have been 6.3 million reported cases and 11000 deaths over the period of one week and a global total of 559 million confirmed cases and 6.3 million deaths reported from the beginning of the outbreak. There was a significant rise in the weekly number of reported cases and death between January 2022 and February 2022. With the development of vaccines and approval for public administration, the numbers have started to decrease. However, WHO recommends that caution should be exerted when interpreting the currently available data. There is a direct correlation between the decreasing number of reported cases and the decreasing number of tests administered globally due to the relaxation of enforcement of public guidelines.

There are three known means of transmission of COVID-19. These are through fomites (commonly used objects that could be contaminated with the pathogen), ballistic droplets (larger particles that travel like a projectile when expelled from the transmitter), and aerosols (smaller particles that remain suspended in air for longer periods of time than ballistic droplets). In the early stages of the COVID-19 outbreak, it was commonly conjectured that the major means of transmission of the disease was through ballistic droplets expelled when a person coughs, sneezes, or talks. This tendency to attribute the spread of a infectious disease mostly to large
droplets is a result of misguided inferences drawn from the works of Carl Flugge in 1897 and Dr. Charles Chapin in the 1910s. Chapin correctly hypothesized that proximity has a significant effect on the transmission of infectious diseases. He then postulated two possibilities for transmission of infections. One is that large droplets can impact a vulnerable person within close proximity and infect said person . Another is that smaller particles could transmit the infections. Chapin could not completely rule out the second possibility. He admitted however that knowledge on the subject of air infection at the time was far too limited. There was more work done on the transmission of infection by large droplets; particularly the work done by Carl Flugge in Germany in the 1890s. So, based on the available evidence at the time, Chapin concluded that infection was spread by spraying droplets. Tuberculosis, one of the highly infectious diseases, was thought of as a disease that is majorly spread through droplets or fomites. However, works by William Wells and Richard Riley in the 20th century undeniably verified that tuberculosis could be transmitted through aerosols. It would later be asserted that tuberculosis could only be transmitted via aerosols as the pathogen needs to be lodged deep in the lungs and this can only be achieved through aerosol transmission. There were similar occurences with measles and chickenpox. The events were similar for COVID-19. However, the occurrence of numerous superspreading events (a few of which are investigated in (Bontempi, 2020; Che Mat, Edinur, Abdul Razab \& Safuan, 2020; Günther, Czech-Sioli, Indenbirken, Robitaille, Tenhaken, Exner, Ottinger, Fischer, Grundhoff \& Brinkmann, 2020)) in which transmitters did not show symptoms such as coughing called for a reevaluation of the relative significance of transmission modes. Marr et al. discuss this in detail in (Marr, Miller, Prather, Haas, Bahnfleth, Corsi, Tang, Herrmann, Pollitt, Ballester \& others, 2021). Tang et al. (Tang, Bahnfleth, Bluyssen, Buonanno, Jimenez, Kurnitski, Li, Miller, Sekhar, Morawska \& others, 2021) summarize what is discussed in (Marr et al., 2021), focusing on clarifying misconceptions about the airborne transmission of the SARS-CoV-2. Randall et al. provide a historical perspective on the consensus of transmission modes of respiratory infectious diseases (Randall, Ewing, Marr, Jimenez \& Bourouiba, 2021). Erroneous notions such as the existence of a clear boundary between 'large' and 'small' particles, a safe distance that people can put between each other, or the inefficiency of masks because of the size of smaller particles are gradually clearing up. However, there are still many uncertainties in the characterization of aerosol and droplet flow. Especially because of the variability in external conditions such as temperature, humidity, and wind speed. Therefore it is important to work towards eliminating these uncertainties.

### 1.2 Prior Works

Numerous works have been done on studying the transmission of particles in various environmental conditions. Anand and Mayya conducted a probabilistic study on the size distribution of virus laden droplets (Anand \& Mayya, 2020). Lee carried out a similar study (Lee, 2020). Lee however attempts to determine a minimum size of the virus-laden particles given the viral load of the transmitter. In both articles, it is stated that small particles have a small probability of being virus-laden (or outright rules out the possibility according to the aerosol generation theory presented in Lee's work). This makes it highly unlikely to inhale a virus-laden particle provided that effective measures are taken against inhaling larger particles. One of the measures commonly suggested is to maintain a 'safe' distance of 2 m to avoid larger particles expelled during sneezing. However, depending on the environmental conditions, even the larger particles can travel well beyond 2 m , thereby extending the safe distance by a considerable size. From Dbouk's and Drikakis' study on coughing and airborne droplet transmission to humans (Dbouk \& Drikakis, 2020), it can be observed that the larger particles can travel beyond 6 m given a wind speed of 4 $\mathrm{km} / \mathrm{h}$. In addition to wind speed playing an important factor in the transmission of pathogens, factors such as temperature, humidity, and exposure time are also important, especially for the spread of smaller particles. Bourouiba (Bourouiba, 2021) showed that multiphase turbulent gas clouds emitted by unprotected coughs or sneezes can carry particles up to 8 m . Considering that smaller particles can remain airbone for extended periods and that the virions can remain active for a minimum of 3 hours, this considerably increases the likelihood of transmission. Chong et al. (Chong, Ng, Hori, Yang, Verzicco \& Lohse, 2021) also demonstrate that smaller particles' effective lifetime can be increased 30 to 150 times more than what is theorized according to Well's model (WELLS, 1934; WELLS \& WELLS, 1936). These smaller droplets remain protected by the turbulent vapor puff emitted during the simulated cough. Ng et al. (Ng, Chong, Yang, Li, Verzicco \& Lohse, 2021) show that depending on the temperature and humidity of the surrounding air, droplets entrained in the vapor puff released after coughing can even grow before shrinking, further increasing the distance they travel and increasing their survivability. In their experiment, Giri et al. (Giri, Biswas, Chase, Xue, Abkarian, Mendez, Saha \& Stone, 2022) explore a mechanism in which respiratory jets released by two conversing individuals can block each other, thereby limiting the transmission of pathogens from one individual to the other. However, there are some limitations in this study, which are rightfully acknowledged. For this phenonema to reliably occur,
the individuals engaging in conversation have to be of similar heights and have to be conversing at short offset intervals. Also, even if the blocking occurs, it increases the lateral spread of the respiratory jets and makes other nearby individuals susceptible to infection.

The ability of the pathogens to survive for extended periods as highlighted in the studies show that the most effective way to limit the spread of the disease is to employ the use of masks in addition to appropriate distancing in well ventilated environments. Bhavsar (Bhavsar, 2021) conducted an experimental study to determine the spread of macroscopic droplets from a simulated cough in a cafeteria setting. He determined that the use of masks and barriers limited the spread of the droplets. Bhavsar makes use of fluorescent paint to simulate the resipiratory droplets and his results are collected immediately after the simulate. This means the results cannot give insight to droplet behaviour over a longer time scale cannot account for virions that remain airborne after the droplets have evaporated.

### 1.3 Research Novelties and Scope

All the studies discussed in the previous section make use of high fidelity 3D Computational Fluid Dynamics (CFD) models or experimental setups. The high fidelity 3D CFD models do produce highly accurate results, but they are computationally expensive and take days to weeks to produce results. The experimental setups on the other hand do produce meaningful results, but they need to be performed in a highly controlled environment and usually have to be repeated multiple times. Due to limitations in computational resources, this research was carried out using a 2D axisymmetric model in COMSOL Multiphysics to model the release of particles from a turbulent jet. The advantage of this method is that simulation results are acquired in considerably less time (longer simulations such as the one done when performing model validation lasted for four hours) and still obtain meaningful results. Admittedly, this model relies on a number of simplifications such as the disregard of the effects of gravity and evaporation. But the results obtained are still meaningful in determining the movement of particles of a range of sizes. Also parameters of the model are set using existing literature so the behaviour of the model is not far off those of the high fidelity 3D models.

In chapter 2, the setup of the simulation (parameters, equations, settings) is ex-
plained and model validation to demonstrate the viability of the results is provided. In chapter 3, the results and insights into the meaning said results are provided. Finally, the thesis is concluded in chapter 4.

## 2. METHODOLOGY

### 2.1 Geometry

The study is carried out on a 2D axisymmetric field. The field domain geometry is presented in Figure 2.1 The field consists of a 2 m by 5 m rectangular domain ( $\mathrm{r}_{1}$ ) which contains a rectangular sub-domain ( $\mathrm{r}_{3}$ ) of size 0.1 m by 0.4 m at the bottom left corner and has a rectangle ( $\mathrm{r}_{2}$ ) of size 0.02 ( $\mathrm{r}_{j e t}$ from Table 2.2 ) m by 0.1 m subtracted from its bottom left corner. The inlet is placed at the top of $r_{2}$ and is given a velocity boundary condition to represent the airflow from the orifice of the transmitter. The outlet is placed at top of $r_{1}$ and is given a pressure boundary condition. Pressure at the outlet is set to static and is given a value of 0 Pa .

### 2.2 Governing Equations

The model consists of Turbulent Flow (k- $\omega$ ), Transport of Diluted Species, and Droplet Sprays in Fluid Flow physics. The governing equations are as follows, with calculations performed locally:

Turbulent Flow
The conservation of momentum equation is given as:

$$
\begin{equation*}
\rho \frac{\partial \mathbf{u}}{\partial t}+\rho(\mathbf{u} \cdot \nabla) \mathbf{u}=\nabla \cdot[-p \mathbf{I}+\mathbf{K}]+\mathbf{F} \tag{2.1}
\end{equation*}
$$

where for the domain fluid (air), $\rho$ is the density, $\mathbf{u}$ is the velocity vector, $\mathbf{K}$ is the


Figure 2.1 Field domain geometry. The 2 m by 5 m rectangular domain is denoted as $\mathrm{r}_{1}$


Figure 2.2 Zoom-in to the bottom left corner of the field domain. The 0.1 m by 0.4 m rectangular sub-domain is denoted as $\mathrm{r}_{2}$. The 0.02 m by 0.1 m rectangle subtracted from the domain is denoted as $\mathrm{r}_{3}$

Table 2.1 Turbulence Model Parameters

| Parameter | Value |
| :---: | :---: |
| $\sigma_{k}^{*}$ | 0.5 |
| $\beta_{0}^{*}$ | 0.09 |
| $\sigma_{w}$ | 0.5 |
| $\alpha$ | 0.52 |
| $\beta_{0}$ | 0.072 |

viscous stress tensor, and F is the volume force vector. $\mathbf{I}$ is the identity matrix.
The continuity (conservation of mass) equation is given as:

$$
\begin{equation*}
\rho \nabla \cdot \mathbf{u}=0 \tag{2.2}
\end{equation*}
$$

where $\rho$ is the density of air and $\mathbf{u}$ is the velocity vector of air.
The viscous stress tensor $\mathbf{K}$ is expressed as:

$$
\begin{equation*}
\mathbf{K}=\left(\mu+\mu_{T}\right)\left(\nabla \mathbf{u}+(\nabla \mathbf{u})^{T}\right) \tag{2.3}
\end{equation*}
$$

where $\mu$ and $\mu_{T}$ are the dynamic viscosity of air and turbulent dynamic viscosity of air respectively. $\mathbf{u}$ is the velocity vector of air.

The $\mathrm{k}-\omega$ turbulence model equations, which solve for k (the turbulent kinetic energy) and $\omega$ (the specific dissipation rate) are:

$$
\begin{equation*}
\rho \frac{\partial k}{\partial t}+\rho(\mathbf{u} \cdot \nabla) k=\nabla \cdot\left[\left(\mu+\mu_{T} \sigma_{k}^{*}\right) \nabla k\right]+P_{k}-\beta_{0}^{*} \rho \omega k \tag{2.4}
\end{equation*}
$$

$$
\begin{equation*}
\rho \frac{\partial \omega}{\partial t}+\rho(\mathbf{u} \cdot \nabla) \omega=\nabla \cdot\left[\left(\mu+\mu_{T} \sigma_{\omega}\right) \nabla \omega\right]+\alpha \frac{\omega}{k} P_{k}-\rho \beta_{0} \omega^{2} \tag{2.5}
\end{equation*}
$$

where $\mathrm{P}_{k}$ is the turbulent kinetic energy source term. $\sigma_{k}^{*}, \beta_{0}^{*}, \sigma_{w}, \alpha$, and $\beta_{0}$ are turbulence model parameters whose values are given in Table 2.1

The turbulent dynamic viscosity, $\mu_{T}$ is expressed in terms of $\rho, \mathrm{k}$, and $\omega$ as:

$$
\begin{equation*}
\mu_{T}=\rho \frac{k}{\omega} \tag{2.6}
\end{equation*}
$$

Table 2.2 Parameters

| Name | Expression | Value | Description |
| :---: | :---: | :---: | :---: |
| $\mathrm{r}_{\text {jet }}$ | 0.02 | 0.02 | Jet radius $(\mathrm{m})$ |
| surft | 0.0729 | 0.0729 | Particle surface tension $(\mathrm{N} / \mathrm{m})$ |
| $\mathrm{T}_{\text {ref }}$ | $273.15+25[\mathrm{~K}]$ | 298.15 K | Reference temperature |
| $\mathrm{p}_{\text {ref }}$ | $1[\mathrm{~atm}]$ | 1.0133 E 5 Pa | Reference pressure level |
| delay | 0 | 0 | Particle release time delay $(\mathrm{s})$ |

The turbulent kinetic energy source term, $\mathrm{P}_{k}$, is expressed as:

$$
\begin{equation*}
P_{k}=\mu_{T}\left[\nabla \mathbf{u}:\left(\nabla \mathbf{u}+(\nabla \mathbf{u})^{T}\right)\right] \tag{2.7}
\end{equation*}
$$

## Transport of Diluted Species

The mass conservation equation for a chemical species is:

$$
\begin{equation*}
\frac{\partial c_{i}}{\partial t}+\nabla \cdot \mathbf{J}_{i}+\mathbf{u} \cdot \nabla c_{i}=R_{i} \tag{2.8}
\end{equation*}
$$

where for the $\mathrm{i}^{\mathrm{t}}$ chemical species (only one is considered in this study), $\mathrm{c}_{i}$ is the concentration ( $\mathrm{mol} / \mathrm{m}^{3}$ ), $\mathrm{J}_{i}$ is the diffusive flux, and $\mathrm{R}_{i}$ is the reaction rate.

The diffusive flux, $\mathrm{J}_{i}$, is given as:

$$
\begin{equation*}
\mathbf{J}_{i}=-D_{i} \nabla c_{i} \tag{2.9}
\end{equation*}
$$

where $\mathrm{D}_{i}$ represents the diffusion coefficient of the $\mathrm{i}^{\text {th }}$ chemical species.

Droplet Sprays in Fluid Flow (Newtonian)
The particles act under the principles of Newton's second law:

$$
\begin{equation*}
m_{p} \frac{d \mathbf{v}}{d t}=\mathbf{F}_{t} \tag{2.10}
\end{equation*}
$$

where for any given particle, $\mathrm{m}_{p}$ is the particle mass, $\mathbf{v}$ is the particle velocity, and $\mathbf{F}_{t}$ is the total force acting on the particle (just drag in this study).

User-defined parameters used in the model are listed in Table 2.2.

### 2.3 Particle Properties

The particles are defined as water droplets of a range of sizes. The size distribution of the particles closely matches the one given in (De Oliveira, Mesquita, Gkantonas, Giusti \& Mastorakos, 2021). Three lognormal distribution functions are defined using the data from (Johnson, Morawska, Ristovski, Hargreaves, Mengersen, Chao, Wan, Li, Xie, Katoshevski \& others, 2011). The lognormal distribution function is expressed as:

$$
\begin{equation*}
f\left(d_{p, 0}\right)=\frac{1}{\sqrt{2 \pi} d_{p, 0} \ln G S D} \exp \left(-\frac{\left(\ln d_{p, 0}-\ln C M D\right)^{2}}{\ln ^{2} G S D}\right) \tag{2.11}
\end{equation*}
$$

where $\mathrm{d}_{p, 0}$ is the particle diameter at release. The GSD, geometric standard deviation and the CMD, count median diameter, are parameters that affect the spread and the median of the lognormal curve.

The parameters of the lognormal distribution functions are outlined in Table 2.3. A total of 5967 particles are released in the ratio 5:7:1 for distributions 1, 2, and 3 respectively. Inertial terms are ignored for distributions 1 and 2 particles. Inertial terms are ignored for the smaller particles because they accelerate over a much smaller time scale compared to the total simulation time (i.e., they have a low Stokes number). The Stokes number, Stk, for a particle in fluid flow is expressed as:

$$
\begin{equation*}
S t k=\frac{\tau_{p}}{\tau_{f}} \tag{2.12}
\end{equation*}
$$

where $\tau_{p}$ is the particle response time and $\tau_{f}$ is the fluid time scale. Due to the nature of turbulent flows, $\tau_{f}$ cannot be assigned a definite value. However, the particle response time, $\tau_{p}$, can be expressed as:

$$
\begin{equation*}
\tau_{p}=\frac{\rho_{p} d_{p}^{2}}{18 \mu_{g}} \tag{2.13}
\end{equation*}
$$

where $\rho_{p}$ is the density of particle, $\mathrm{d}_{p}$ is the particle diameter, and $\mu_{g}$ is the dynamic viscosity of the surrounding fluid. $\tau_{p}$ is directly proportional to $\mathrm{d}_{p}^{2}$, so the aerosols, which are about 2-3 orders of magnitude smaller than the droplets, have Stokes numbers that are about 4-6 orders of magnitude smaller than those of the droplets.

The initial particle velocity is set to the velocity at the inlet at the time the particle is released. The particles lose momentum over time when drag force due to the

Table 2.3 Lognormal Distribution Function Parameters

| Distribution | 1 | 2 | 3 |
| :---: | :---: | :---: | :---: |
| Count Median Diameter $(\mu \mathrm{m})$ | 1.6 | 1.7 | 123 |
| Geometric Standard Deviation | 1.25 | 1.68 | 1.837 |

difference between particle velocity and surrounding airflow velocity acts on the particles.

The velocity profile of the cough is given in Figure 2.3. The velocity profile is obtained from (Dudalski et al., 2020). Dudalski et al. calculated the cough velocity profile using parameters and formulations provided in (Gupta, Lin \& Chen, 2009). Gupta et al. describe the flow characteristics using non-dimensional parameters. They non-dimensionalize the flow rate using Cough Peak Flow Rate (CPFR) and they non-dimensionalize the time using Peak Velocity Time (PVT). The nondimensional flow rate, $\bar{M}$, and the non-dimensional time, $\tau$, are expressed as:

$$
\begin{equation*}
\bar{M}=\frac{\text { Flowrate }}{C P F R} \tag{2.14}
\end{equation*}
$$

$$
\begin{equation*}
\tau=\frac{\text { Time }}{P V T} \tag{2.15}
\end{equation*}
$$

The non-dimensional flow rate, $\bar{M}$, is also expressed as:

$$
\begin{equation*}
\bar{M}=\frac{a_{1} \tau^{b_{1}-1} \exp \left(-\frac{\tau}{c_{1}}\right)}{\Gamma\left(b_{1}\right) c_{1}^{b_{1}}}, \text { for } \tau<1.2 \tag{2.16}
\end{equation*}
$$

$$
\begin{equation*}
\bar{M}=\frac{a_{1} \tau^{b_{1}-1} \exp \left(-\frac{\tau}{c_{1}}\right)}{\Gamma\left(b_{1}\right) c_{1}^{b_{1}}}+\frac{a_{2}(\tau-1.2)^{b_{2}-1} \exp \left(-\frac{\tau-1.2}{c_{2}}\right)}{\Gamma\left(b_{2}\right) c_{2}^{b_{2}}}, \text { for } \tau \geq 1.2 \tag{2.17}
\end{equation*}
$$

where $\mathrm{a}_{1}=1.680, \mathrm{~b}_{1}=3.338, \mathrm{c}_{1}=0.428$, and:

$$
\begin{equation*}
a_{2}=\frac{C E V}{P V T \times C P F R}-a_{1} \tag{2.18}
\end{equation*}
$$

$$
\begin{equation*}
b_{2}=\frac{-2.158 \times C E V}{P V T \times C P F R}+10.457 \tag{2.19}
\end{equation*}
$$



Figure 2.3 Velocity profile of the cough at the inlet. y-axis: Velocity [m/s], x axis: Time [s]. Data obtained from (Dudalski et al., 2020)

$$
\begin{equation*}
c_{2}=\frac{1.8}{b_{2}-1} \tag{2.20}
\end{equation*}
$$

$\Gamma$ is the gamma function, which is expressed as:

$$
\begin{equation*}
\Gamma(x)=(x-1)! \tag{2.21}
\end{equation*}
$$

For the purpose of analyzing the effect of inlet velocity on different metrics (covered in Chapter 3), the cough velocity profile is adjusted by changing the velocity magnitude (maximum inlet velocity ( $\mathrm{v}_{\text {peak }}$ ) ranges from $11 \mathrm{~m} / \mathrm{s}$ to $22 \mathrm{~m} / \mathrm{s}$ ). The particles are released at 5 ms intervals for the first 0.25 seconds of the cough. The release duration of the particles were determined using results from (Bahl, de Silva, MacIntyre, Bhattacharjee, Chughtai \& Doolan, 2021). Each lognormal distribution set is released from separate 3 by 3 rectangular grids placed close to the inlet. The particles are released from grids instead of directly at the inlet to avoid simulation failure brought about by having numerous wall interactions at the inlet. Phenomena such as evaporation and breakup are ignored. Breakup is ignored because the Weber number (We), the ratio of drag force to surface tension force, for all droplets
is significantly small. The Weber number of a water droplet is expressed as:

$$
\begin{equation*}
W e=\frac{\rho U_{r e l}^{2} r}{\sigma} \tag{2.22}
\end{equation*}
$$

where $\rho$ is the density of the droplet, $\mathrm{U}_{\text {rel }}$ is the relative velocity between the droplet and the surrounding fluid, r is the radius of the droplet, and $\sigma$ is the surface tension of the droplet. Assuming all other parameters are constant, the Weber number is directly proportional to the size of the droplet. Even for the largest droplets generated by the model (size on the order of $700 \mu \mathrm{~m}$ ) and assuming maximum $\mathrm{U}_{\text {rel }}$ $(22 \mathrm{~m} / \mathrm{s})$, the Weber number is significantly less than 1. According to (Strotos, Malgarinos, Nikolopoulos \& Gavaises, 2016), breakup of droplets reliably occurs at around $\mathrm{We}=13$. This phenomenon is termed as bag breakup. Breakups can occur at lower Weber numbers between 1 and 13, but these breakups occur due to oscillations of the droplets, happen occasionally, and result in about 2 or 3 droplets (comparable in size to the parent droplet) forming from each parent droplet. Because the Weber number for all droplets is significantly less than 1, breakup of the droplets can effectively be ruled out.

Evaporation is ignored because the larger droplets do not evaporate significantly in the considered timeframe. Depending on the relative humidity, the smaller aerosols can evaporate in a matter of seconds. However, because COMSOL treats the particles as homogeneous, evaporation of the particles beyond a specified cutoff diameter results in elimination of the particles. Also, because the study focuses on the transmission of viral load, neglecting evaporation to keep the particle volumes constant allows for the particle volume to be directly related to the viral load.

### 2.4 Numerical Approach

The advection of the particles is simulated using incompressible Reynolds-Averaged Navier Stokes (RANS) equations. The k- $\omega$ turbulence model is applied with the turbulent intensity set to the default value (0.05) specified in COMSOL and the turbulent length scale set to 0.0015 . According to COMSOL's documentation of turbulent flow, fully turbulent flows generally have intensities between 0.05 and 0.1 , and the turbulent length scale can be set to 0.075 L , where L is the jet half-width (jet radius) for an axisymmetric jet.


Figure 2.4 The field used in COMSOL and its mesh layout

The time step for output results is set to 0.005 s for the range $[0,0.095] \mathrm{s}, 0.05$ s for the range $[0.1,0.95] \mathrm{s}$, and 0.5 for the range $[1,120] \mathrm{s}$. This time-stepping ensures that the dynamics of the flow and particle motion are properly captured while reducing the data size of the results by a considerable amount.The variables are solved for in two studies. The first study solves for the turbulent flow variables and diffusion of the diluted species variables, whereas the second study solves for the particle dynamics using priorly established flow results from the first study. The first study uses a segregated approach to solve for the variables, while the second study uses a fully coupled approach.

### 2.4.1 Mesh Settings

Triangular meshes populate the entire field with meshes of a higher refinement placed in the region between rectangles r 2 and r 3 . The meshes in the region between r 2 and r 3 have a maximum element size of $0.004 \mathrm{~m}\left(\mathrm{r}_{\text {jet }} / 5\right)$ whereas the meshes in the region between r 3 and r 1 have a maximum element size of $0.06 \mathrm{~m}\left(3^{*} \mathrm{r}_{j e t}\right)$. The field and its mesh layout is presented in Figures 2.4 and 2.5.


Figure 2.5 Zoom-in of the field, focusing on the region between r2 and r3. Higher refinement meshes are placed in this region

### 2.5 Model Validation

For the model validation, parameters of the model were set up to closely match the experiment done in 2000 by Antoine et al.(Antoine et al., 2001) The inlet velocity was set to a constant value for all times. The velocity was set so that the flow at the inlet has a Reynold's number of 10000 , as in the experiment. The background co-flow velocity was set to 0.05 times the inlet velocity, as done in the experiment. A new inlet was defined at the lower boundary of $r 1$ to introduce background flow. The simulation time was set to 20 seconds. This provides enough time for the flow to fully develop across the entire domain. The model results as compared to the experimental data are presented in Figures 2.6-2.9. As can be seen in Figure 2.6, for the streamwise distribution of the longitudinal velocity, the model result closely matches the experimental data. However, as can be seen in Figure 2.7-2.9, for the radial distribution of the logitudinal velocity, the model results start to deviate from the experimental data at points farther away from the centerline of the jet. These deviations become more pronounced at points farther away from the jet in the streamwise direction. These deviations arise from finite field approximation errors.

The MATLAB script used to perform model validation can be found in Appendix A.

Turbulent Jet Model Validation - Streamwise Distribution of Longitudinal Velocity


Figure 2.6 Validation results of turbulent jet model: streamwise distribution of longitudinal velocity. - : COMSOL k- $\omega$ model; • : Experimental data from (Antoine et al., 2001)


Figure 2.7 Validation results of turbulent jet model: radial distribution of longitudinal velocity at $\mathrm{x} / \mathrm{d}=80$. - : COMSOL $\mathrm{k}-\omega$ model; • : Experimental data from (Antoine et al., 2001)


Figure 2.8 Validation results of turbulent jet model: radial distribution of longitudinal velocity at $\mathrm{x} / \mathrm{d}=110$. - : COMSOL $\mathrm{k}-\omega$ model; •: Experimental data from (Antoine et al., 2001)


Figure 2.9 Validation results of turbulent jet model: radial distribution of longitudinal velocity at $\mathrm{x} / \mathrm{d}=120$. - : COMSOL $\mathrm{k}-\omega$ model; •: Experimental data from (Antoine et al., 2001)

### 2.6 Result Metrics

Definitions of the metrics used in chapter 3 (Results) are found in this section. These metrics are used for particles or diluted species mass that have travelled beyond a line/plane which is a specified target distance in front of the transmitter. The metrics are:

## 1. Size Distribution of Particles:

This is a frequency distribution of the number of particles within a particular size range that have travelled beyond a specified target distance. The size ranges increase exponentially. Results are presented in the form of 3D bar charts. Normalized size distributions (bar heights adding up to 1) are also provided to better depict the evolution of the size distribution of particles with respect to time.

## 2. Fraction of Expired Particle Volume:

The expired particle volume is the sum of the volumes of all the particles released by the transmitter. The fraction of expired particle volume is a measure of the proportion of the expired particle volume that has travelled beyond a specified target distance. Fraction of expired particle volume is expressed in the result figures as $\frac{\Sigma V_{p}}{V_{0}}$, where $\mathrm{V}_{p}$ is the volume of a particle that has travelled beyond a specified target distance and $V_{0}$ is the expired particle volume at the inlet.

Given that the volume of each particle does not change in this study, the fraction of expired particle volume is directly related to the fraction of the total viral load emitted by the transmitter. The volume of each particle remaining constant means that particle volume and particle mass are interchangeable.

## 3. Fraction of Expired Diluted Species Mass:

The expired diluted species mass is the total mass of the diluted species released by the transmitter. The fraction of expired diluted species mass is a measure of the proportion of the expired diluted species mass that has travelled beyond a specified target distance. Fraction of expired diluted species mass is expressed in the result figures as $\frac{\Sigma M_{s}}{M_{0}}$, where $\Sigma \mathrm{M}_{s}$ is the total mass of the species that has travelled beyond a specific target distance and $\mathrm{M}_{0}$ is the expired diluted species mass at the inlet.

Given that the mass is directly related to the number of moles of the dilutes species, the fraction of expired diluted species mass for a specified target distance ( $z_{\text {target }}$ )
can be calculated as:

$$
\begin{equation*}
\text { Fraction of expired diluted species mass }=\frac{\int_{z_{\text {target }}}^{5} \int_{0}^{2} 2 \pi r c(r, z)\left(z>z_{\text {target }}\right) d r d z}{\int_{0.1}^{5} \int_{0}^{2} 2 \pi r c(r, z) d r d z} \tag{2.23}
\end{equation*}
$$

where $\mathrm{c}(\mathrm{r}, \mathrm{z})$ is the concentration of the diluted species at coordinate ( $\mathrm{r}, \mathrm{z}$ ). The expression $\mathrm{z}>\mathrm{z}_{\text {target }}$ is equal to 1 when the expression is true and 0 when the expression is false.

## 4. Cumulative Radial Distribution of Accumulated Particle Volume:

For a specified target distance, the accumulated particle volume is the sum of the volume of all the particles that have travelled beyond the target distance. To obtain the radial distribution, from which the cumulative radial distribution can be obtained, the exact coordinates at which particles cross the target distance boundary are needed. To calculate these coordinates, the positions of the particles are recorded for the moments just before and after they cross the target boundary. Then linear interpolation is performed to estimate the coordinates at which the particles cross the target distance boundary. Once these coordinates are obtained, the radial distribution of accumulated particle volume is calculated by determining the fraction of the accumulated particle volume that crosses the target distance boundary within a certain radial range. For the results presented, the radial ranges are each sized 1 mm . The cumulative radial distribution is calculated by adding the fractions of the accumulated particle volumes up to a certain radial range. The cumulative radial distribution is expressed in the result figures as $\frac{\Sigma V_{p}}{V_{\text {accum }}}$ where $V_{p}$ is the volume of a particle that has travelled beyond a specified target distance and $\mathrm{V}_{\text {accum }}$ is the sum of the volumes of all the particles that have travelled beyond the target distance.

The MATLAB script used to calculate all the metrics discussed here can be found in Appendix A.

## 3. RESULTS

The following results help to elucidate the temporal and spatial evolution of the size distribution of the ejected particles. Most of the results presented here are cover a range of cough velocities (maximum inlet velocities ( $\mathrm{v}_{\text {peak }}$ ) of $11 \mathrm{~m} / \mathrm{s}, 16.5$ $\mathrm{m} / \mathrm{s}$, and $22 \mathrm{~m} / \mathrm{s}$ ). Definitions of the metrics used in this chapter are provided in the 'Result Metrics' section of Chapter 2. The results can be used to assess risk of infection in terms of viral load. According to (De Oliveira et al., 2021), a viral load of $10^{4}-10^{9}$ copies $/ \mathrm{ml}$ can be found in the sputum and throat swabs of sick individuals. The viral load can rarely go as high as $10^{10}$ copies $/ \mathrm{ml}$. A quantum is defined as the amount of viral load required to be inhaled to have a probability of transmission of $63 \%$. According to (Dhand \& Li, 2020), a cough produces about 3000 droplets. Given that the simulation uses about 6000 droplets and the calculated total volume of the droplets is about $1.65 \mathrm{e}-8 \mathrm{~m}^{3}(1.65 \mathrm{e}-2 \mathrm{ml})$, the approximate volume of droplets expelled during a cough would be $0.825 \mathrm{e}-2 \mathrm{ml}$. Assuming a viral load of $10^{9}$ copies $/ \mathrm{ml}$ from the transmitter, a total of about 8.25 e 6 copies is released from a cough. According to (Prentiss, Chu \& Berggren, 2022), the amount of viral load for a quantum of SARS-CoV-2 is on the order of 600 copies (virions). This means that an invidual has to receive effectively 0 percent of a cough to mitigate the risk of infection.

### 3.1 Size Distribution of Particles vs. Time

Figures 3.1- 3.18 show how the size distribution of the particles that reach a target location ( $\mathrm{z}_{\text {particle }}>\mathrm{z}_{\text {target }}$ ) evolves with time. Results are presented (in a pair of figures) for different target distances and different cough velocities. For each pair of figures, the first depicts the total count of the particles grouped into several particle size bins while the second depicts the normalized size distribution (bin heights add


Figure 3.1 Time evolution of size distribution of particles that have reached a target distance of 2 m in front the transmitter. Cough $v_{\text {peak }}=11 \mathrm{~m} / \mathrm{s}$
up to 1) of the particles. The size of the particle size bins increases exponentially and the size axis scales logarithmically. Although the simulation results cover a duration of 120 s , data is truncated in the figures because the count and the normalized size distribution of the particles undergo negligible (if any) change for later times. As can be observed from these figures, the larger particles reach the target locations at faster than the smaller particles do. This is to be expected as the larger ballistic particles have a larger inertia and do not decelerate as quickly as the smaller particles. Because the larger particles arrive at the target distances faster than the smaller particles do, the initial size distributions closely match the lognormal distribution of distribution 3 particles. This distribution can be seen in the initial times of Figure 3.16 . As the smaller particles begin to arrive at the target location, the size distribution rapidly changes to match the distribution found in Figure 3.13.

### 3.2 Fraction of Expired Particle Volume vs. Distance

Figures 3.19-3.21 show, for different cough velocities, the fraction of the expired particle volume at the inlet that can be found beyond a target distance measured at different time stamps. The horizontal part of the curves for the later times at


Figure 3.2 Time evolution of normalized size distribution of particles that have reached a target distance of 2 m in front the transmitter. Cough $v_{\text {peak }}=11 \mathrm{~m} / \mathrm{s}$


Figure 3.3 Time evolution of size distribution of particles that have reached a target distance of 3 m in front the transmitter. Cough $v_{\text {peak }}=11 \mathrm{~m} / \mathrm{s}$


Figure 3.4 Time evolution of normalized size distribution of particles that have reached a target distance of 3 m in front the transmitter. Cough $v_{\text {peak }}=11 \mathrm{~m} / \mathrm{s}$


Figure 3.5 Time evolution of size distribution of particles that have reached a target distance of 4 m in front the transmitter. Cough $v_{\text {peak }}=11 \mathrm{~m} / \mathrm{s}$


Figure 3.6 Time evolution of normalized size distribution of particles that have reached a target distance of 4 m in front the transmitter. Cough $v_{\text {peak }}=11 \mathrm{~m} / \mathrm{s}$


Figure 3.7 Time evolution of size distribution of particles that have reached a target distance of 2 m in front the transmitter. Cough $v_{\text {peak }}=16.5 \mathrm{~m} / \mathrm{s}$


Figure 3.8 Time evolution of normalized size distribution of particles that have reached a target distance of 2 m in front the transmitter. Cough $v_{\text {peak }}=16.5 \mathrm{~m} / \mathrm{s}$


Figure 3.9 Time evolution of size distribution of particles that have reached a target distance of 3 m in front the transmitter. Cough $v_{\text {peak }}=16.5 \mathrm{~m} / \mathrm{s}$


Figure 3.10 Time evolution of normalized size distribution of particles that have reached a target distance of 3 m in front the transmitter. Cough $v_{\text {peak }}=16.5 \mathrm{~m} / \mathrm{s}$


Figure 3.11 Time evolution of size distribution of particles that have reached a target distance of 4 m in front the transmitter. Cough $v_{\text {peak }}=16.5 \mathrm{~m} / \mathrm{s}$


Figure 3.12 Time evolution of normalized size distribution of particles that have reached a target distance of 4 m in front the transmitter. Cough $v_{p e a k}=16.5 \mathrm{~m} / \mathrm{s}$


Figure 3.13 Time evolution of size distribution of particles that have reached a target distance of 2 m in front the transmitter. Cough $v_{\text {peak }}=22 \mathrm{~m} / \mathrm{s}$


Figure 3.14 Time evolution of normalized size distribution of particles that have reached a target distance of 2 m in front the transmitter. Cough $v_{\text {peak }}=22 \mathrm{~m} / \mathrm{s}$


Figure 3.15 Time evolution of size distribution of particles that have reached a target distance of 3 m in front the transmitter. Cough $v_{\text {peak }}=22 \mathrm{~m} / \mathrm{s}$


Figure 3.16 Time evolution of normalized size distribution of particles that have reached a target distance of 3 m in front the transmitter. Cough $v_{\text {peak }}=22 \mathrm{~m} / \mathrm{s}$


Figure 3.17 Time evolution of size distribution of particles that have reached a target distance of 4 m in front the transmitter. Cough $v_{\text {peak }}=22 \mathrm{~m} / \mathrm{s}$


Figure 3.18 Time evolution of normalized size distribution of particles that have reached a target distance of 4 m in front the transmitter. Cough $v_{\text {peak }}=22 \mathrm{~m} / \mathrm{s}$
the farther distances could indicate that the larger particles that travel ballistically and do not decelerate rapidly enough to be captured by the plume released from the jet account for roughly 20 percent of the total particle volume for cough $\mathrm{v}_{\text {peak }}$ $=11 \mathrm{~m} / \mathrm{s}, 37$ percent of the total particle volume for cough $\mathrm{v}_{\text {peak }}=16.5 \mathrm{~m} / \mathrm{s}$, and 47 percent of the total particle volume for cough $\mathrm{v}_{\text {peak }}=22 \mathrm{~m} / \mathrm{s}$. This increase in percentage with increasing inlet velocity could be attributed to the decrease in drag experienced by the particles as a result of the increase in surrounding airflow velocity (which is affected by inlet velocity).

### 3.3 Fraction of Expired Particle Volume vs. Time

Figures 3.22-3.24 depict how the portion of the expired particle volume at the inlet that has reached various target distances changes with time. The graph was made to scale logarithmically on the time axis to better capture the changes that occur rapidly on smaller time scales and become more gradual on larger time scales. It can be observed that, for the timescale considered in the simulations, all the particles travel at least 3.0 m in front of the transmitter for $\mathrm{v}_{\text {peak }}=11 \mathrm{~m} / \mathrm{s}$, and 3.6 m for $\mathrm{v}_{\text {peak }}=16.5 \mathrm{~m} / \mathrm{s}$ and $22 \mathrm{~m} / \mathrm{s}$. For all cough velocities, 4.2 m remains a safe target


Figure 3.19 Plots of the fraction of total particle volume released at the inlet that have traveled a target distance vs. target distance. Cough $\mathrm{v}_{\text {peak }}=11 \mathrm{~m} / \mathrm{s}$. Individual curves represent the data captured at different time stamps


Figure 3.20 Plots of the fraction of total particle volume released at the inlet that have traveled a target distance vs. target distance. Cough $\mathrm{v}_{\text {peak }}=16.5 \mathrm{~m} / \mathrm{s}$. Individual curves represent the data captured at different time stamps


Figure 3.21 Plots of the fraction of total particle volume released at the inlet that have traveled a target distance vs. target distance. Cough $\mathrm{v}_{\text {peak }}=22 \mathrm{~m} / \mathrm{s}$. Individual curves represent the data captured at different time stamps
distance for less than a second. For $\mathrm{v}_{\text {peak }}=22 \mathrm{~m} / \mathrm{s}$, the smaller particles begin to arrive at 4.2 m at least 30 seconds after release. This can be observed from the sharp rise in the fraction of expired particle volume at this time in Figure 3.24. For $\mathrm{v}_{\text {peak }}=11 \mathrm{~m} / \mathrm{s}$, the smaller particles begin to arrive at 4.2 m at about 100 seconds after release.

### 3.4 Fraction of Expired Diluted Species Mass vs. Time

Figures 3.25-3.27 show the portion of the expired diluted species mass measured against time. These results are used for comparison with the results presented in Figures 3.22-3.24. Mass is used instead of the volume for the diluted species because the volume of the diluted species continually increases as a result of diffusion. In addition, the concentration of species varies across the entire field. The diffusion coefficient of the diluted species is set to $6.3 \mathrm{e}-6 \mathrm{~m}^{2} / \mathrm{s}$. This value is based on the diffusion coefficient of gas-phase nicotine as specified in (Eatough, Benner, Bayona, Richards, Lamb, Lee, Lewis \& Hansen, 1989). The time profile of the concentration at the inlet is a pulse which lasts for the entire duration of the cough. In contrast


Figure 3.22 Plots of the fraction of total particle volume released at the inlet that have traveled a set target distance vs. time. Cough $\mathrm{v}_{\text {peak }}=11 \mathrm{~m} / \mathrm{s}$. Individual curves represent the data for different target distances


Figure 3.23 Plots of the fraction of total particle volume released at the inlet that have traveled a set target distance vs. time. Cough $\mathrm{v}_{\text {peak }}=16.5 \mathrm{~m} / \mathrm{s}$. Individual curves represent the data for different target distances


Figure 3.24 Plots of the fraction of total particle volume released at the inlet that have traveled a set target distance vs. time. Cough $\mathrm{v}_{\text {peak }}=22 \mathrm{~m} / \mathrm{s}$. Individual curves represent the data for different target distances
to the particle volume plot presented previously, there is a smoother progression of the diluted species mass curves with time. Figure 3.28-3.36 present a comparison between the expired particle volume curve and the diluted species mass curve at different target distances. Their mass fractions are compared because the mass of the particles is proportional to the volume of the particles. Because the larger particles move ahead of the plume due to their higher inertia, the fraction of expired particle volume at the target distance is always higher than that of the expired diluted species mass for the same time instance. It can be noted that at the times the particle curves reach their maxima, the diluted species curves begin to flatten. This is because the smaller particles tend to be entrained within the cough plume. This entrainment of the smaller particles in the cough plume means that the movement of the smaller particles could be somewhat inferred from the diluted species curves.

### 3.5 Cumulative Radial Distribution of Accumulated Particle Volume

Figures 3.37-3.39 shows the cumulative radial distribution of accumulated particle volume at a target distance of 3 m . It can be observed from the figures that for all


Figure 3.25 Plots of the fraction of total diluted species mass released at the inlet that have traveled a set target distance vs. time. Cough $\mathrm{v}_{\text {peak }}=11 \mathrm{~m} / \mathrm{s}$. Individual curves represent the data for different target distances

Plots of Fraction of Expired Diluted Species Mass vs. Time, Cough $v_{\text {peak }}=16.5 \mathrm{~m} / \mathrm{s}$


Figure 3.26 Plots of the fraction of total diluted species mass released at the inlet that have traveled a set target distance vs. time. Cough $\mathrm{v}_{\text {peak }}=16.5 \mathrm{~m} / \mathrm{s}$. Individual curves represent the data for different target distances


Figure 3.27 Plots of the fraction of total diluted species mass released at the inlet that have traveled a set target distance vs. time. Cough $\mathrm{v}_{\text {peak }}=22 \mathrm{~m} / \mathrm{s}$. Individual curves represent the data for different target distances


Figure 3.28 Plots of the fraction of total mass released at the inlet that have traveled a set target distance vs. time. Comparison between particles plot and diluted species plot for the same target distance


Figure 3.29 Plots of the fraction of total mass released at the inlet that have traveled a set target distance vs. time. Comparison between particles plot and diluted species plot for the same target distance


Figure 3.30 Plots of the fraction of total mass released at the inlet that have traveled a set target distance vs. time. Comparison between particles plot and diluted species plot for the same target distance


Figure 3.31 Plots of the fraction of total mass released at the inlet that have traveled a set target distance vs. time. Comparison between particles plot and diluted species plot for the same target distance


Figure 3.32 Plots of the fraction of total mass released at the inlet that have traveled a set target distance vs. time. Comparison between particles plot and diluted species plot for the same target distance


Figure 3.33 Plots of the fraction of total mass released at the inlet that have traveled a set target distance vs. time. Comparison between particles plot and diluted species plot for the same target distance


Figure 3.34 Plots of the fraction of total mass released at the inlet that have traveled a set target distance vs. time. Comparison between particles plot and diluted species plot for the same target distance


Figure 3.35 Plots of the fraction of total mass released at the inlet that have traveled a set target distance vs. time. Comparison between particles plot and diluted species plot for the same target distance


Figure 3.36 Plots of the fraction of total mass released at the inlet that have traveled a set target distance vs. time. Comparison between particles plot and diluted species plot for the same target distance


Figure 3.37 Plots of the cumulative radial distribution of the fraction of total particle volume accumulated at the target distance. Cough $\mathrm{v}_{\text {peak }}=11 \mathrm{~m} / \mathrm{s}$. Individual curves represent the data for different target distances
cough velocities, all the particles that crossed the targets of $1.0 \mathrm{~m}, 2.0 \mathrm{~m}$, and 3.0 m did so within about $0.1 \mathrm{~m}, 0.3 \mathrm{~m}$, and 0.5 m from the axis of symmetry (centerline of the jet), respectively. This implies a somewhat constant spread angle of the particles within a quiescent environment. According to (Dudalski et al., 2020), this corresponds to a spread angle ( $\theta$ ) of about $22.6^{\circ}$, which is well within the range of their results. In Figure 3.37, all the particles that crossed the target of 4.0 m did so within less than 0.1 m from the centerline of the jet. This is because for the cough $\mathrm{v}_{\text {peak }}$ of $11 \mathrm{~m} / \mathrm{s}$, only the large ballistic droplets travelled as far as 4.0 m for the duration of the simulation, . In Figures 3.38 and 3.39, the particles spread as far as 0.7 m from the centerline of the jet, corresponding with the spread angle of $22.6^{\circ}$ mentioned earlier. A constant spread angle suggests that inhalation of viral load from the transmitter in the short term can largely be avoided by staying out of the line of sight of the transmitter.

### 3.6 Effect of Background Wind



Figure 3.38 Plots of the cumulative radial distribution of the fraction of total particle volume accumulated at the target distance. Cough $\mathrm{v}_{\text {peak }}=16.5 \mathrm{~m} / \mathrm{s}$. Individual curves represent the data for different target distances


Figure 3.39 Plots of the cumulative radial distribution of the fraction of total particle volume accumulated at the target distance. Cough $\mathrm{v}_{\text {peak }}=22 \mathrm{~m} / \mathrm{s}$. Individual curves represent the data for different target distances


Figure 3.40 Change in the field domain geometry to introduce background flow. The arc of a quarter circle of radius 0.1 m connects the edge of the cough inlet to the background flow inlet boundary

To study the effect of background wind on the flow of the particles and the accumulation of viral load, background winds of velocities $0.2 \mathrm{~m} / \mathrm{s}, 0 / 6 \mathrm{~m} / \mathrm{s}$, and $1.0 \mathrm{~m} / \mathrm{s}$ that move in the same direction as the cough plume are put into effect. Background wind is applied for the cough with the lowest velocity ( $\mathrm{v}_{\text {peak }}=11 \mathrm{~m} / \mathrm{s}$ ). The background wind is applied from the bottom of the 2D axisymmetric field (rectangle $\mathrm{r}_{1}$ ). Particle release and flow at the cough inlet are delayed by 0.1 s to allow the background flow to fully develop. To ensure a smoother flow around the boundary, the arc of a quarter circle of radius 0.1 m is introduced to connect the cough transmitter inlet and the lower boundary. The revised field domain geometry is presented in Figure 3.40.

Fraction of Expired Particle Volume vs. Time plots are presented in Figures 3.41 - 3.43. It should be noted that because the initial release time of the particles is 0.1 s , there is a time shift in the plots. This effect is negligible for latter times. It can be observed that even with a background wind speed of $0.2 \mathrm{~m} / \mathrm{s}$, all the particles reach a target distance of 4.2 m at about 10 seconds after release. There is a significant decrease in the time required to reach the target distance compared to the time required in a static background (about 100 seconds). This highlights the effect of background flow on the transmission of viral load.


Figure 3.41 Plots of the fraction of total particle volume released at the inlet that have traveled a set target distance vs. time. Cough $\mathrm{v}_{\text {peak }}=11 \mathrm{~m} / \mathrm{s}$. Background flow of $0.2 \mathrm{~m} / \mathrm{s}$ applied. Individual curves represent the data for different target distances


Figure 3.42 Plots of the fraction of total particle volume released at the inlet that have traveled a set target distance vs. time. Cough $\mathrm{v}_{\text {peak }}=11 \mathrm{~m} / \mathrm{s}$. Background flow of $0.6 \mathrm{~m} / \mathrm{s}$ applied. Individual curves represent the data for different target distances


Figure 3.43 Plots of the fraction of total particle volume released at the inlet that have traveled a set target distance vs. time. Cough $\mathrm{v}_{\text {peak }}=11 \mathrm{~m} / \mathrm{s}$. Background flow of $1 \mathrm{~m} / \mathrm{s}$ applied. Individual curves represent the data for different target distances

## 4. CONCLUSION

After doing research and adjusting parameters, validation of the turbulent jet flow model used was performed by setting the fluid properties to match the nondimensional parameters of the fluid used in the experiment done by Antoine et al. (Antoine et al., 2001). The results from the turbulent jet model used in this study were then compared with Antoine et al.'s experimental data. There were some deviations, but this is most likely due to finite field approximation errors.

The results presented in this thesis focus on the space and time progression of the droplet/aerosol particle. The particles' size distribution and their spatial distribution are emphasized in the results. Some simplifications were made for the simulations. One is that the effect of gravity on the particles were not considered. This is not a problem for the smaller particles, but the model assumes that the larger particles remain airborne along with the smaller particles. While this is not the case, this does not detract from the implications of the results and the statistical inferences that can be drawn from them. For the largest of particles considered (size on the order of $700 \mu \mathrm{~m}$ ), and the lowest speed ( $11 \mathrm{~m} / \mathrm{s}$ ), the drag force and gravitational force can be calculated as:

$$
\begin{equation*}
F_{d}=6 \pi \mu R v \tag{4.1}
\end{equation*}
$$

$$
\begin{equation*}
F_{g}=m g=\rho g V \tag{4.2}
\end{equation*}
$$

where $\mathrm{F}_{d}$ is the drag force, $\mu$ is the dynamic viscosity of air (about $18.37 \mu \mathrm{~Pa} . \mathrm{s}$ ), $R$ is the radius of the particle, $v$ is the relative velocity between the particle and the surrounding fluid (about $11 \mathrm{~m} / \mathrm{s}$ ), $F_{g}$ is the gravitational force, $\rho$ is the density of the particle (water), $g$ is the acceleration due to gravity, and $V$ is the volume of the particle. The resulting forces are on the same order of magnitude ( $\mathrm{F}_{d}=1.333 \mu \mathrm{~N}$, $\left.\mathrm{F}_{g}=1.7618 \mu \mathrm{~N}\right)$. Assuming the downwards acceleration remains constant, the larger particles fall from a height of 1.7 m in about 0.6 seconds. According to Figure 3.22,
for a $\mathrm{v}_{\text {peak }}$ of $11 \mathrm{~m} / \mathrm{s}$, the larger particles begin to arrive at a target distance of 4.2 m in that time. According to Figure 3.24, more of the larger particles arrive at a target distance of 4.2 m in that time. The results can be used as a statistical reference for the movement of the particles in free space. A more complex analysis on the distribution of the particles taking settling time of the particles into consideration could be performed, but that is beyond the scope of this research.

The second simplification is that evaporation of the droplets/aerosols is not taken into consideration. Given that COMSOL models particle as homogeneous, and that evaporation of the particles would mean elimination of the particles from the study, the neglect of evaporation of the particles was a necessary concession to make. This concession is also necessary because the particles are assumed to have a constant viral load density, and the results emphasize the accumulation of particle volume, which directly corresponds to viral load, at a target location.

One important result from this study is that each of the groups of larger and smaller particles has a certain timescale in which they reach target distances. As they reach the target distances, the distribution stays relatively consistent with the initial distribution of all the particles released by the transmitter.

Another important result is that in a static environment, all of the particles can be found in a conical region with a spread angle of about $22.6^{\circ}$. This means that for the short term, inhalation of viral load released by the transmitter can largely be avoided by staying out of the line of sight of the transmitter.

One more important result is that background wind can significantly aid the transmission of particles. As seen in Figure 3.22, smaller particles can take up to 100 seconds to reach a target distance of 4.2 m . It can be observed from Figure 3.41 that with a background wind speed of $0.2 \mathrm{~m} / \mathrm{s}$, all of the particles are transported to the target distance of 4.2 m in about 10 seconds.

Given that a cough has much more than the viral load needed to reliably infect a person, and that the background condition is almost never truly static, in addition to maintaining 'safe' distances, employing the use of masks and shields is recommended for the mitigation of the transmission of viral load.

The results obtained here can be improved in time with the development of more sophisticated models, but they are still important for understanding the nature of movement of particles.

### 4.1 Future Work

Future works to be done on this study involve making use of more complex models. To include the effect on gravity on the particles, the results of the 2 D axisymmetric model can be imported into a 3D model by rotating the domain about the axis of symmetry. Gravitational forces can then be added to the particles.

Studies that can be done separately or collectively are the study on the advection of smaller particles (distributions 1 and 2 particles) and the effect of filtration on the transmission of particles. Given that larger particles can reach the ground from a height of 1.7 m in a fraction of a second, and face masks are effective in filtering out larger particles, a study can be performed solely on the advection of the smaller particles to quantify how much viral load can potentially reach a target. For a study on the effect of filtration on the transmission of particles, further research would have to be conducted on current methods used. One proposition would be to model the mask as a porous media.

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## APPENDIX A

## MATLAB Codes

The MATLAB Codes used to compile all of the results presented in this study are given below.

```
close all
clear
clc
load partpos_cough1_60.mat % particle position data
load partsize_cough1_60.mat % particle size data
load conc_table_cough1_60.mat % diluted species concentration data
G_array = G_array'; % contains position data
H_array = H_array'; % contains size data
C_array = C_array'; % contains mol. data
target = 2.0; % target distance
size_dist_time = 5; % end time for figures 2 and 3
partcount = 0; % number of particles that reach target distance
v_peak = 22; % peak velocity of cough profile
% edges1 = 0:10e-6:700e-6;
edges2 = zeros(1,42); % bin edges for particle size distribution
time1 = 10;
time2 = 30;
time3 = 60;
time4 = 120;
increment1 = 0.005; % time increments (steps) for different time ranges
increment2 = 0.05;
increment3 = 0.5;
index1 = (time1/increment3 + 37) * 2 + 1; %adjusted according to the structure
    of position data
index2 = (time2/increment3 + 37) * 2 + 1;
index3 = (time3/increment3 + 37) * 2 + 1;
index4 = (time4/increment3 + 37) * 2 + 1;
for y = 2:length(edges2)
    edges2(y) = (1.1835^(y-1))*(1e-6); % bin size increases exponentially
end
figtitle = ['Particles that have travelled at least ',num2str(target), ' m in
    front of the Transmitter, Cough v_{peak} = ', num2str(v_peak)];
for group = 1:4
    B_array = H_array;
    if group == 1
            A_array = G_array(1:index1,:);
    elseif group == 2
            A_array = G_array(1:index2,:);
    elseif group == 3
            A_array = G_array(1:index3,:);
    else
```

```
    A_array = G_array(1:index4,:);
    end
    Asize = size(A_array);
    Bsize = size(B_array);
    partcount = 0;
    for y = 1:Asize(2)
    for x = 3:2:Asize(1)
        if A_array(x,y) >= target
                partcount = partcount + 1;
                break
        end
        end
    end
    disp(partcount)
    part = zeros(1,partcount);
    k=1;
    for y = 1:Asize(2)
    for x = 3:2:Asize(1)
            if A_array (x,y) >= target
                part(k) = B_array(Bsize(1),y);
                k = k+1;
                break
        end
    end
    end
    figure(1)
    subplot(2,2,group)
    %histogram(part, edges2)
    histogram(part,edges2,'Normalization','probability')
    ylim([0 1])
    grid on
    set(gca,'xscale','log')
    set(gca,'GridLineStyle','-')
    set(gca,'YMinorGrid','on')
    set(gca,'GridAlpha',0.3)
    %set(gca,'MinorGridLineStyle','-')
    if group == 1
    if partcount == 1
        title1 = ['Distribution after ', num2str(time1), ' Seconds -
',num2str(partcount),' Particle'];
        %title1 = ['Distribution at Emitter Location at Time of Emission -
',num2str(partcount),' Particle'];
        title(title1)
    else
        title1 = ['Distribution after ', num2str(time1), ' Seconds -
',num2str(partcount),' Particles'];
                %title1 = ['Distribution at Emitter Location at Time of Emission -
',num2str(partcount),' Particle'];
        title(title1)
        end
    elseif group == 2
        if partcount == 1
```

```
    title2 = ['Distribution after ', num2str(time2), ' Seconds -
    ',num2str(partcount),' Particle'];
            title(title2)
        else
            title2 = ['Distribution after ', num2str(time2), ' Seconds -
    ',num2str(partcount),' Particles'];
            title(title2)
        end
    elseif group == 3
        if partcount == 1
        title3 = ['Distribution after ', num2str(time3), ' Seconds -
    ',num2str(partcount),' Particle'];
        title(title3)
            else
            title3 = ['Distribution after ', num2str(time3), ' Seconds -
    ',num2str(partcount),' Particles'];
            title(title3)
            end
        else
            if partcount == 1
            title4 = ['Distribution after ', num2str(time4), ' Seconds -
    ',num2str(partcount),' Particle'];
            title(title4)
            else
            title4 = ['Distribution after ', num2str(time4), ' Seconds -
',num2str(partcount),' Particles'];
            title(title4)
            end
    end
    ylabel('Number of Particles')
    xlabel('Size (m)')
end
figure(1)
sgtitle(figtitle)
Z1 = zeros(length(edges2)-1,120);
Z2 = zeros(length(edges2)-1,120);
%----------------------------------------------------------------
% Calculation of Size Distributtion of Particles vs. Time
for time=1:120
    index = (time/increment3 + 37) * 2 + 1; % data index for given time
    Y_array = H_array; % size data
    X_array = G_array(1:index,:); %position data up to specified time
    Ysize = size(Y_array);
    Xsize = size(X_array);
    partcount = 0;
    for y = 1:Xsize(2)
        for x = 3:2:Xsize(1)
            if X_array(x,y) >= target
                partcount = partcount + 1; %increase partcount if particles is
    found beyond the target distance
                break
```

```
                    end
            end
    end
    part = zeros(1,partcount);
    k=1;
    for y = 1:Xsize(2)
        for x = 3:2:Xsize(1)
            if X_array (x,y) >= target
                part(k) = Y_array(Ysize(1),y); %store the sizes of all
particles that reached target distance
                k = k+1;
                break
            end
        end
    end
    count = zeros(1,length(edges2)-1);
    for x = 1:length(count)
        for y = 1:partcount
            if part(y) <= edges2(x+1) && part(y) > edges2(x)
                count(x) = count(x) + 1; % if particle is in size range, add
to bin count
            end
        end
    end
    dist = count/partcount; %normalize distribution by partcount
    Z1(:,time) = count;
    Z2(:,time) = dist;
end
yAxis = edges2(1:10:length(edges2)-1)*1e6;
%sprintf('yMin: %5f yMax: %5f', [min(yAxis) max(yAxis)])
figure(2)
b = bar3(Z1(:,1:size_dist_time));
figtitle = ['Number of Particles that have traveled at least
    ',num2str(target),' m in front of the Trasmitter, Cough v_{peak} = ',
    num2str(v_peak), ' m/s'];
%title(figtitle)
xlabel('Time [s]')
ylabel('Size [\mum]')
zlabel('Count')
set(gca,'YTick',[[0 10 20 30 40])
% for k = 1:length(b)
% zdata = b (k).zData;
% b(k).CData = zdata;
    b(k).FaceColor = 'interp';
end
% set(gca,'YTickLabel',yAxis)
for k = 1:size_dist_time
    zdata = b(k).ZData;
    b(k).CData = zdata;
```

```
    b(k).FaceColor = 'interp';
end
yaxiscell = get(gca,'YTickLabel');
yaxis = zeros(size(yaxiscell));
for y = 2:length(yaxiscell)
    yaxis (y) = edges2(2)*1.1835^((40/(length(yaxis) - 1))*(y-1)-1)*1e6;
end
set(gca,'YTickLabel',yaxis)
figure(3)
b = bar3(Z2(:,1:size_dist_time));
figtitle = ['Normalized Distribution of Particles that have traveled at
    least ',num2str(target),' m in front of the Trasmitter, Cough v_{peak} = ',
    num2str(v_peak), ' m/s'];
%title(figtitle)
xlabel('Time [s]')
ylabel('Size [\mum]')
zlabel('PDF')
set(gca,'YTick',[[0 10 20 30 40])
% for k = 1:length(b)
% zdata = b(k).zData;
% b(k).CData = zdata;
% b(k).FaceColor = 'interp';
% end
% set(gca,'YTickLabel',yAxis)
for k = 1:size_dist_time
    zdata = b(k).zData;
    b(k).CData = zdata;
    b(k).FaceColor = 'interp';
end
set(gca,'YTickLabel',yaxis)
%--------------------------------------------------------
% Calculations of Fraction of Expired Particle Volume vs. Distance
% & Fraction of Expired Particle Volume vs. Time
distance = 0:0.01:5;
times = [0:0.005:0.095 0.1:0.05:0.95 1:0.5:120];
totalVol = 0; % Expired Particle Volume
targetVol0_3 = zeros(size(distance)); %accumulated particle volume vs.
    distance data at different timestamps
targetVol0_5 = zeros(size(distance));
targetVol1 = zeros(size(distance));
targetVol5 = zeros(size(distance));
targetVol10 = zeros(size(distance));
targetVol30 = zeros(size(distance));
targetVol60 = zeros(size(distance));
targetVol120 = zeros(size(distance));
%G_array_no_nan = G_array;
%G_array_no_nan(isnan(A_array_no_nan)) = 0;
for y = 1:Bsize(2)
```

```
    totalVol = totalVol + (4/3)*pi*B_array(Bsize(1),y)^3;
end
i=1;
for target2 = distance
    for timesd =[[0.3 0.5 1 5 10 30 60 120]
        if timesd < 0.1
            index = (timesd/increment1 + 1) * 2 + 1; % index of timestamps
    according to particle position dats
        elseif timesd < 1
            index = (timesd/increment2 + 19) * 2 + 1;
        else
            index = (timesd/increment3 + 37) * 2 + 1;
        end
        target_cumul_vol = 0; %total volume of particles that have reached a
    target distance
        for y = 1:Asize(2)
            for x = 3:2:index
                    if A_array (x,y) >= target2
                        target_cumul_vol = target_cumul_vol +
    (4/3)*pi*B_array(Bsize(1),y)^3;
                                    break
                    end
            end
        end
        if timesd == 10
            targetVol10(i) = target_cumul_vol;
            elseif timesd == 30
            targetVol30(i) = target_cumul_vol;
            elseif timesd == 60
            targetVol60(i) = target_cumul_vol;
            elseif timesd == 5
            targetVol5(i) = target_cumul_vol;
            elseif timesd == 1
            targetVol1(i) = target_cumul_vol;
            elseif timesd == 0.5
            targetVol0_5(i) = target_cumul_vol;
            elseif timesd == 0.3
                targetVol0_3(i) = target_cumul_vol;
            else
            targetVol120(i) = target_cumul_vol;
            end
    end
    i = i+1;
end
targetVol0_3_portion = targetVol0_3/totalVol; %fraction of expired particle
    volume vs. distance data at different timestamps
targetVol0_5_portion = targetVol0_5/totalVol;
targetVoll_portion = targetVoll/totalVol;
targetVol5_portion = targetVol5/totalVol;
targetVol10_portion = targetVol10/totalVol;
targetVol30_portion = targetVol30/totalVol;
targetVol60_portion = targetVol60/totalVol;
```

```
targetVol120_portion = targetVol120/totalVol;
timeVol1 = zeros(size(times)); %accumulated particle volume vs. time data at
    different target distances
timeVol2 = zeros(size(times));
timeVol3 = zeros(size(times));
timeVol4 = zeros(size(times));
timeVol5 = zeros(size(times));
timeVol6 = zeros(size(times));
timeVol7 = zeros(size(times));
i = 1;
for times2 = times
        if times2 < 0.1
            index = (times2/increment1 + 1) * 2 + 1;
        elseif times2 < 1
            index = (times2/increment2 + 19) * 2 + 1;
        else
            index = (times2/increment3 + 37) * 2 + 1;
        end
        for group = 1:7
            target3 = group*0.6;
            time_cumul_vol = 0;
            for y = 1:Asize(2)
                for x = 3:2:index
                    if A_array(x,y) >= target3
                                    time_cumul_vol = time_cumul_vol +
    (4/3)*pi*B_array(Bsize(1),y)^3;
                                    break
                    end
            end
            end
            if group == 1
                timeVol1(i) = time_cumul_vol;
            elseif group == 2
                timeVol2(i) = time_cumul_vol;
            elseif group == 3
                timeVol3(i) = time_cumul_vol;
            elseif group == 4
                timeVol4(i) = time_cumul_vol;
            elseif group == 5
                timeVol5(i) = time_cumul_vol;
            elseif group == 6
                timeVol6(i) = time_cumul_vol;
            else
                timeVol7(i) = time_cumul_vol;
            end
        end
        i = i+1;
end
timeVoll_portion = timeVoll/totalVol; %fraction of expired particle volume vs.
    time data at different target distances
```

```
timeVol2_portion = timeVol2/totalVol;
timeVol3_portion = timeVol3/totalVol;
timeVol4_portion = timeVol4/totalVol;
timeVol5_portion = timeVol5/totalVol;
timeVol6_portion = timeVol6/totalVol;
timeVol7_portion = timeVol7/totalVol;
figure(4)
plot(distance,targetVol0_3_portion,'DisplayName','Time = 0.3
    s','Marker','o','MarkerSize',6,'MarkerIndices',1:25:length(distance),'LineWidth',2)
figtitle = ['Plots of Fraction of Expired Particle Volume vs. Distance, Cough
    v_{peak} = ', num2str(v_peak), ' m/s'];
title(figtitle)
hold on
grid on
plot(distance,targetVol0_5_portion,'DisplayName','Time = 0.5
    s','Marker','v','MarkerSize',6,'MarkerIndices',1:25:length(distance),'LineWidth',2)
plot(distance,targetVol1_portion,'DisplayName','Time = 1
    s','Marker','^','MarkerSize',6,'MarkerIndices',1:25:length(distance),'LineWidth',2)
plot(distance,targetVol5_portion,'DisplayName','Time = 5
    s','Marker','|','MarkerSize',8,'MarkerIndices',1:10:length(distance),'LineWidth',2)
plot(distance,targetVol10_portion,'DisplayName','Time = 10
    s','Marker','s','MarkerSize',6,'MarkerIndices',1:25:length(distance),'LineWidth',2)
plot(distance,targetVol30_portion,'DisplayName','Time = 30
    s','Marker','.','MarkerSize',20,'MarkerIndices',1:25:length(distance),'LineWidth',2)
plot(distance,targetVol60_portion,'DisplayName','Time = 60
    s','Marker','*','MarkerSize',8,'MarkerIndices',1:25:length(distance),'LineWidth',2)
plot(distance,targetVol120_portion,'DisplayName','Time = 120 s','LineWidth',2)
xlabel('Distance [m]')
ylabel('$\frac{\Sigma V_p}{V_0}$','Interpreter','latex','FontSize',25)
legend
figure(5)
semilogx(times,timeVol1_portion,'DisplayName','Target = 0.6 m','LineWidth',2)
figtitle = ['Plots of Fraction of Expired Particle Volume vs. Time, Cough
    v_{peak} = ', num2str(v_peak), ' m/s'];
title(figtitle)
hold on
grid on
semilogx(times,timeVol2_portion,'DisplayName','Target = 1.2
    m','Marker','^','MarkerSize',6,'MarkerIndices',1:5:length(times),'LineWidth',2)
semilogx(times,timeVol3_portion,'DisplayName','Target = 1.8
    m','Marker','|','MarkerSize',8,'MarkerIndices',1:5:length(times),'LineWidth',2)
semilogx(times,timeVol4_portion,'DisplayName','Target = 2.4
    m','Marker','v','MarkerSize',6,'MarkerIndices',1:5:length(times),'LineWidth',2)
semilogx(times,timeVol5_portion,'DisplayName','Target = 3.0
    m','Marker','.','MarkerSize',20,'MarkerIndices',1:5:length(times),'LineWidth',2)
semilogx(times,timeVol6_portion,'DisplayName','Target = 3.6
    m','Marker','s','MarkerSize',8,'MarkerIndices',1:20:length(times),'LineWidth',2)
semilogx(times,timeVol7_portion,'DisplayName','Target = 4.2
    m','Marker','*','MarkerSize',8,'MarkerIndices',1:10:length(times),'LineWidth',2)
xlabel('Time [s]')
ylabel('$\frac{\Sigma V_p}{V_0}$','Interpreter','latex','FontSize',25)
legend('Location','southeast')
```


## Calculation of Fraction of Expired Diluted Species Mass vs. Time

```
C_array_allconc = C__array(2:size(C_array,1),1:size(C_array,2));
```

C_array_conc $=$ C_array (3:size (C_array, 1), 1:size(C_array, 2)) ; \% mol. data for
target distances
C_array_norm $=$ C_array_conc/max(max(C_array_allconc)); \% normalized mol. data
$=$ fraction of expired diluted species mass

## figure(6)

semilogx (times, C_array_norm(1,:),'DisplayName','Target $=0.6 \mathrm{~m}$ ', 'LineWidth', 2 )
figtitle $=$ ['Plots of Fraction of Expired Diluted Species Mass vs. Time, Cough
v__\{peak\} $=$ ', num2str(v_peak), ' m/s'];
title(figtitle)
\%title('Fraction of Expired Diluted Species Mass vs. Time, Cough v_\{peak\} $=22$ m/s')
hold on
grid on
semilogx (times, C_array_norm (2, :) ,'DisplayName','Target =1.2
m','Marker', '+','MarkerSize', 8,'MarkerIndices', 1:15:length(times), 'LineWidth', 2)
semilogx (times, C_array_norm (3, :), 'DisplayName','Target $=1.8$
$\left.m^{\prime}, ' M a r k e r ', ' \wedge ', ' M a r k e r S i z e ', 8, ' M a r k e r I n d i c e s ', 1: 10: l e n g t h(t i m e s), ' L i n e W i d t h ', 2\right)$
semilogx (times, C_array_norm (4, :), 'DisplayName','Target $=2.4$

semilogx (times, C_array_norm (5, :), 'DisplayName','Target $=3.0$
$\left.m^{\prime}, ' M a r k e r ', ' . ', ' M a r k e r S i z e ', 20, ' M a r k e r I n d i c e s ', 1: 10: l e n g t h(t i m e s), ' L i n e W i d t h ', 2\right)$
semilogx (times, C_array_norm (6, :) ,'DisplayName','Target $=3.6$
m', 'Marker', 's','MarkerSize', 8, 'MarkerIndices', 1:10:length(times), 'LineWidth', 2)
semilogx (times, C_array_norm (7, :),'DisplayName','Target = 4.2
 xlabel('Time [s]')
Ylabel ('\$ $\mathrm{frac}\left\{\backslash\right.$ Sigma M_s $\left\{\begin{array}{l}\text { M_0 }\end{array}\right.$
\%ylabel('Fraction of Expired Mass')
legend('Location', 'northwest')
$x \lim \left(\left[\begin{array}{ll}0 & 120\end{array}\right)\right.$

\% Comparison between Fraction of Expired Particle Volume and Fraction of
\% Expired Diluted Species Mass
timeVol_part_portion $=$ timeVol5_portion; \% Fraction of Expired Particle \% Volume vs. Time data
time_conc_portion $=$ C_array_norm(5, :); \% Fraction of Expired Diluted \% Mass vs. Time data
figure (7)
semilogx(times,timeVol_part_portion, 'DisplayName', 'Particles', 'LineWidth', 2)
hold on
grid on
semilogx(times,time_conc_portion, 'DisplayName', 'Diluted
Species','Marker','.','MarkerSize', 20,'MarkerIndices', 1:10:length(times),'LineWidth',2)
xlabel('Time [s]')
ylabel ('\$\frac\{\Sigma M_\{p,s\}\}\{M_0\}\$','Interpreter', 'latex','FontSize', 25)

```
%ylabel('Fraction of Expired Mass')
text = ['Plots of Fraction of Expired Mass vs. Time, Cough v_{peak} = ',
    num2str(v_peak), ' m/s , Target = 3.0 m'];
title(text)
legend('Location','northwest')
xlim([0 120])
%------------------------------------------------------------------------------------
% Calculation of Cumulative Radial Distribution of Accumulated Volume of
% Particles
dr = 0.001; % radial range size
rk = dr:dr:1.0;
Vk1 = zeros(size(rk)); % cumulative radial distribution of accumulated
Vk2 = zeros(size(rk)); % volume for each target distance
Vk3 = zeros(size(rk));
Vk4 = zeros(size(rk));
target_i = 1; % target distances
target_ii = 2;
target_iii = 3;
target_iv = 4;
% calculation of coordinate each particle passes through
for y = 1:Asize(2)
    for x = 3:2:Asize(1)
        if A_array(x,y) >= target_iii
            if A_array(x,y) == target_iii
                r = A_array (x-1,y);
            else % linear interpolation for calculation of r
                r = (A_array (x-1,y)*(target_iii-A_array (x-2,y)) +
    A_array (x-3,y) * (A_array (x,y) -target_iii))/(A_array (x,y) -A_array (x-2,y));
            end
            for i = 1:size(rk,2)
                if r <= rk(i)
                                    Vk3(i) = Vk3(i) + (4/3)*pi*B_array(Bsize(1),y)^3;
                                    %break
                end
            end
            break
        end
    end
end
for y = 1:Asize(2)
    for x = 3:2:Asize(1)
        if A_array(x,y) >= target_i
            if A_array(x,y) == target_i
                r = A_array (x-1,y);
            else
                    r=(A_array (x-1,y)* (target_i-A_array (x-2,y)) +
    A_array (x-3,y) * (A_array (x,y) -target_i)) /(A_array (x,y) -A_array (x-2,y));
        end
        for i = 1:size(rk, 2)
            if r <= rk(i)
```

```
                    Vk1(i) = Vk1(i) + (4/3)*pi*B_array(Bsize(1),y)^3;
                    %break
                        end
                end
                break
            end
    end
end
for y = 1:Asize(2)
    for x = 3:2:Asize(1)
        if A_array(x,y) >= target_ii
                if A_array (x,y) == target_ii
                    r = A_array(x-1,y);
        else
            r = (A_array(x-1,y)*(target_ii-A_array(x-2,y)) +
        A_array (x-3,y)*(A_array (x,y)-target_ii))/(A_array (x,y)-A_array (x-2,y));
            end
                for i = 1:size(rk,2)
            if r <= rk(i)
                    Vk2(i) = Vk2(i) + (4/3)*pi*B_array(Bsize(1),y)^3;
                        %break
            end
                end
                break
            end
        end
end
for y = 1:Asize(2)
    for x = 3:2:Asize(1)
        if A_array(x,y) >= target_iv
            if A_array(x,y) == target_iv
                r = A_array(x-1,y);
            else
            r = (A_array (x-1,y)* (target_iv-A_array (x-2,y)) +
    A_array (x-3,y)*(A_array (x,y) -target_iv))/(A_array (x,y) -A_array (x-2,y));
            end
            for i = 1:size(rk,2)
                    if r <= rk(i)
                                    Vk4(i) = Vk4(i) + (4/3)*pi*B_array(Bsize(1),y)^3;
                                    %break
                    end
            end
            break
            end
    end
end
Vk3 = Vk3/max(Vk3); % distribution normalized by total accumulated volume
Vk1 = Vk1/max(Vk1);
Vk2 = Vk2/max (Vk2);
Vk4 = Vk4/max(Vk4);
```

```
%rk = flip(rk);
%Vk = flip(Vk);
figure(8)
plot(rk,Vk1,'DisplayName','Target = 1.0 m','LineWidth',2)
grid on
hold on
plot(rk,Vk2,'DisplayName','Target = 2.0
    m','Marker','.','MarkerSize',20,'MarkerIndices',1:20:length(rk),'LineWidth',2)
plot(rk,Vk3,'DisplayName','Target = 3.0
    m','Marker','*','MarkerSize',8,'MarkerIndices',1:20:length(rk),'LineWidth',2)
plot(rk,Vk4,'DisplayName','Target = 4.0
    m','Marker','|','MarkerSize',8,'MarkerIndices',1:20:length(rk),'LineWidth',2)
text = ['Cumulative Radial Distribution of Accumulated Volume of Particles,
    v_{peak} = ', num2str(v_peak), ' m/s'];
title(text)
xlabel('Distance from axis of symmetry [m]')
ylabel('$\frac{\Sigma V_p}{V_{accum}}$','Interpreter','latex','FontSize',25)
legend('Location','southeast')
```

Model validation
\% Streamwise Distribution of Longitudinal Velocity
turb_jet_val_stream = load('turb_jet_val_stream.txt'); \% model data
turb_jet_exp_stream = load('turb_jet_exp_streamwise_U0_over_Um.csv');
\%experimental data
figure (9)
plot(turb_jet_val_stream(:,1),turb_jet_val_stream(:, 2),'DisplayName','COMSOL
k-\omega model','LineWidth',2)
hold on
grid on
plot (turb_jet_exp_stream(:,1),turb_jet_exp_stream(:,2),'DisplayName','Antoine
et. al (2001)','LineStyle','none','Marker','o','MarkerFaceColor','r')
legend
title('Turbulent Jet Model Validation - Streamwise Distribution of
Longitudinal Velocity')
xlabel('x/d')
ylabel('\$\frac\{\bar\{U\}_0\}\{\bar\{U\}_m\}\$','Interpreter','latex','FontSize', 25)
\% Radial Distribution of Longitudinal Velocity at $x / d=80$
turb_jet_val_radial_xd_80 = load('turb_jet_val_rad_xd_80.txt');
turb_jet_exp_radial_xd_80 = load('turb_jet_exp_radial_U_over_Um_xd_80.csv');
figure (10)
plot (turb_jet_val_radial_xd_80(:,1),turb_jet_val_radial_xd_80(:,2), 'DisplayName', 'COMSOL
k-\omega model','LineWidth',2)
hold on
grid on
plot (turb_jet_exp_radial_xd_80(:,1),turb_jet_exp_radial_xd_80(:,2), 'DisplayName', 'Antoine
et. al (2001)','LineStyle','none','Marker','o','MarkerFaceColor','r')
legend
title('Turbulent Jet Model Validation - Radial Distribution of Longitudinal
Velocity $\left.(x / d=80)^{\prime}\right)$

```
xlabel('r/x')
ylabel('$\frac{\bar{U}}{\bar{U}_m}$','Interpreter','latex','FontSize',25)
% Radial Distribution of Longitudinal Velocity at x/d = 110
turb_jet_val_radial_xd_110 = load('turb_jet_val_rad_xd_110.txt');
turb_jet_exp_radial_xd_110 = load('turb_jet_exp_radial_U_over_Um_xd_110.csv');
figure(11)
plot(turb_jet_val_radial_xd_110(:,1),turb_jet_val_radial_xd_110(:,2),'DisplayName','COMSOI
    k-\omega model','LineWidth',2)
hold on
grid on
plot(turb_jet_exp_radial_xd_110(:,1),turb_jet_exp_radial_xd_110(:,2),'DisplayName','Antoin
    et. al (2001)','LineStyle','none','Marker','o','MarkerFaceColor','r')
legend
title('Turbulent Jet Model Validation - Radial Distribution of Longitudinal
    Velocity (x/d = 110)')
xlabel('r/x')
ylabel('$\frac{\bar{U}}{\bar{U}_m}$','Interpreter','latex','FontSize',25)
% Radial Distribution of Longitudinal Velocity at x/d = 120
turb_jet_val_radial_xd_120 = load('turb_jet_val_rad_xd_120.txt');
turb_jet_exp_radial_xd_120 = load('turb_jet_exp_radial_U_over_Um_xd_120.csv');
figure(12)
plot(turb_jet_val_radial_xd_120(:,1),turb_jet_val_radial_xd_120(:,2),'DisplayName','COMSOL
    k-\omega model','LineWidth',2)
hold on
grid on
plot(turb_jet_exp_radial_xd_120(:,1),turb_jet_exp_radial_xd_120(:,2),'DisplayName','Antoin
    et. al (2001)','LineStyle','none','Marker','o','MarkerFaceColor','r')
legend
title('Turbulent Jet Model Validation - Radial Distribution of Longitudinal
    Velocity (x/d = 120)')
xlabel('r/x')
ylabel('$\frac{\bar{U}}{\bar{U}_m}$','Interpreter','latex','FontSize',25)
```


## Published with MATLAB® R2022a

```
% Effect of Background Wind
load partpos_cough3_60_tailwind_0_2.mat % particle position data for
                                    % different wind speeds
load partpos_cough3__60_tailwind__0_6.mat
load partpos_cough3_60_tailwind_1.mat
load partsize_cough3_60_tailwind_0_2.mat % particle size data for different
    % wind speeds
load partsize_cough3_60_tailwind_0_6.mat
load partsize_cough3__60_tailwind__1.mat
G1_array = G1_array'; % contains position data for 0.2 m/s background flow
G2_array = G2_array'; % contains position data for 0.6 m/s background flow
G3_array = G3_array'; % contains position data for 1 m/s background flow
H1_array = H1_array'; % contains size data for 0.2 m/s background flow
H2_array = H2_array'; % contains size data for 0.6 m/s background flow
H3_array = H3_array'; % contains size data for 1 m/s background flow
totalVol_0_2 = 0;
totalVol_0_6 = 0;
totalVol_1 = 0;
for y = 1:size(H1_array,2)
    totalVol_0_2 = totalVol_0_2 + (4/3)*pi*H1_array(size(H1_array,1),y)^3;
    totalVol_0_6 = totalVol_0_6 + (4/3)*pi*H2_array(size(H2_array,1),y)^3;
    totalVol_1 = totalVol_1 + (4/3)*pi*H3_array(size(H3_array,1),y)^3;
end
timeVol1_0_2 = zeros(size(times)); %accumulated particle volume vs. time data
    at different target distances for 0.2 m/s background flow
timeVol2_0_2 = zeros(size(times));
timeVol3_0_2 = zeros(size(times));
timeVol4_0_2 = zeros(size(times));
timeVol5_0_2 = zeros(size(times));
timeVol6_0_2 = zeros(size(times));
timeVol7_0_2 = zeros(size(times));
timeVol1_0_6 = zeros(size(times)); %accumulated particle volume vs. time data
    at different target distances for 0.6 m/s background flow
timeVol2_0_6 = zeros(size(times));
timeVol3_0_6 = zeros(size(times));
timeVol4_0_6 = zeros(size(times));
timeVol5_0_6 = zeros(size(times));
timeVol6_0_6 = zeros(size(times));
timeVol7_0_6 = zeros(size(times));
timeVol1_1 = zeros(size(times)); %accumulated particle volume vs. time data at
    different target distances for 1 m/s background flow
timeVol2_1 = zeros(size(times));
```

```
timeVol3_1 = zeros(size(times));
timeVol4_1 = zeros(size(times));
timeVol5_1 = zeros(size(times));
timeVol6_1 = zeros(size(times));
timeVol7_1 = zeros(size(times));
i = 1;
for times2 = times
    if times2 < 0.1
        index = (times2/increment1 + 1) * 2 + 1;
    elseif times2 < 1
        index = (times2/increment2 + 19) * 2 + 1;
    else
            index = (times2/increment3 + 37) * 2 + 1;
    end
    for group = 1:7
        target4 = group*0.6;
        time_cumul_vol_0_2 = 0;
        time_cumul_vol_0_6 = 0;
        time_cumul_vol_1 = 0;
        for y = 1:size(G1_array,2)
            search_G1_array = 1;
            search_G2_array = 1;
            search_G3_array = 1;
            for x = 3:2:index
                    if G1_array(x,y) >= target4
                                    if search_G1_array == 1
                                    time_cumul_vol_0_2 = time_cumul_vol_0_2 +
(4/3)*pi*H1_array(size(H1_array,1),y)^3;
                                    search_G1_array = 0;
                                    end
    end
    if G2_array(x,y) >= target4
                            if search_G2_array == 1
                                    time_cumul_vol_0_6 = time_cumul_vol_0_6 +
    (4/3)*pi*H2_array(size(H2_array,1),y)^3;
                                    search_G2_array = 0;
                                    end
            end
            if G3_array(x,y) >= target4
                if search_G3_array == 1
                time_cumul_vol_1 = time_cumul_vol_1 +
(4/3)*pi*H3_array(size(H3_array,1),y)^3;
                search_G3_array = 0;
                end
            end
        end
    end
    if group == 1
        timeVol1_0_2(i) = time_cumul_vol_0_2;
        timeVol1_0_6(i) = time_cumul_vol_0_6;
        timeVol1_1(i) = time_cumul_vol_1;
```

```
        elseif group == 2
        timeVol2_0_2(i) = time_cumul_vol_0_2;
        timeVol2_0_6(i) = time_cumul_vol_0_6;
        timeVol2_1(i) = time_cumul_vol_1;
        elseif group == 3
        timeVol3_0_2(i) = time_cumul_vol_0_2;
        timeVol3_0_6(i) = time_cumul_vol_0_6;
        timeVol3_1(i) = time_cumul_vol_1;
        elseif group == 4
        timeVol4_0_2(i) = time_cumul_vol_0_2;
        timeVol4_0_6(i) = time_cumul_vol_0_6;
        timeVol4_1(i) = time_cumul_vol_1;
        elseif group == 5
        timeVol5_0_2(i) = time_cumul_vol_0_2;
        timeVol5_0_6(i) = time_cumul_vol_0_6;
        timeVol5_1(i) = time_cumul_vol_1;
        elseif group == 6
            timeVol6_0_2(i) = time_cumul_vol_0_2;
            timeVol6_0_6(i) = time_cumul_vol_0_6;
            timeVol6_1(i) = time_cumul_vol_1;
        else
            timeVol7_0_2(i) = time_cumul_vol_0_2;
            timeVol7_0_6(i) = time_cumul_vol_0_6;
            timeVol7_1(i) = time_cumul_vol_1;
        end
    end
    i = i+1;
end
timeVol1_portion_0_2 = timeVol1_0_2/totalVol_0_2; %fraction of expired
    particle volume vs. time data at different target distances
timeVol1_portion_0_6 = timeVol1_0_6/totalVol_0_6;
timeVol1_portion_1 = timeVol1_1/totalVol_1;
timeVol2_portion_0_2 = timeVol2_0_2/totalVol_0_2;
timeVol2_portion_0_6 = timeVol2_0_6/totalVol_0_6;
timeVol2_portion_1 = timeVol2_1/totalVol_1;
timeVol3_portion_0_2 = timeVol3_0_2/totalVol_0_2;
timeVol3_portion_0_6 = timeVol3_0_6/totalVol_0_6;
timeVol3_portion_1 = timeVol3_1/totalVol_1;
timeVol4_portion_0_2 = timeVol4_0_2/totalVol_0_2;
timeVol4_portion_0_6 = timeVol4_0_6/totalVol_0_6;
timeVol4_portion_1 = timeVol4_1/totalVol_1;
timeVol5_portion_0_2 = timeVol5_0_2/totalVol_0_2;
timeVol5_portion_0_6 = timeVol5_0_6/totalVol_0_6;
timeVol5_portion_1 = timeVol5_1/totalVol_1;
```

```
timeVol6_portion_0_2 = timeVol6_0_2/totalVol_0_2;
timeVol6_portion_0_6 = timeVol6_0_6/totalVol_0_6;
timeVol6_portion_1 = timeVol6_1/totalVol_1;
timeVol7_portion_0_2 = timeVol7_0_2/totalVol_0_2;
timeVol7_portion_0_6 = timeVol7_0_6/totalVol_0_6;
timeVol7_portion_1 = timeVol7_1/totalVol_1;
figure(9)
semilogx(times,timeVol1_portion_0_2,'DisplayName','Target = 0.6
    m','LineWidth',2)
figtitle = ['Plots of Fraction of Expired Particle Volume vs. Time, Cough
    v_{peak} = ', num2str(v_peak), ' m/s, background wind speed of 0.2 m/s'];
title(figtitle)
hold on
grid on
semilogx(times,timeVol2_portion_0_2,'DisplayName','Target = 1.2
    m','Marker','^','MarkerSize',6,'MarkerIndices',1:5:length(times),'LineWidth',2)
semilogx(times,timeVol3_portion_0_2,'DisplayName','Target = 1.8
    m','Marker','|','MarkerSize',8,'MarkerIndices',1:5:length(times),'LineWidth',2)
semilogx(times,timeVol4_portion_0_2,'DisplayName','Target = 2.4
    m','Marker','v','MarkerSize',6,'MarkerIndices',1:5:length(times),'LineWidth',2)
semilogx(times,timeVol5_portion_0_2,'DisplayName','Target = 3.0
    m','Marker','.','MarkerSize',20,'MarkerIndices',1:5:length(times),'LineWidth',2)
semilogx(times,timeVol6_portion_0_2,'DisplayName','Target = 3.6
    m','Marker','s','MarkerSize',8,'MarkerIndices',1:20:length(times),'LineWidth',2)
semilogx(times,timeVol7_portion_0_2,'DisplayName','Target = 4.2
    m','Marker','*','MarkerSize',8,'MarkerIndices',1:10:length(times),'LineWidth',2)
xlabel('Time [s]')
ylabel('$\frac{\Sigma V_p}{V_0}$','Interpreter','latex','FontSize',25)
legend('Location','southeast')
xlim([0 120])
figure(10)
semilogx(times,timeVol1_portion_0_6,'DisplayName','Target = 0.6
    m','LineWidth',2)
figtitle = ['Plots of Fraction of Expired Particle Volume vs. Time, Cough
    v_{peak} = ', num2str(v_peak), ' m/s, background wind speed of 0.6 m/s'];
title(figtitle)
hold on
grid on
semilogx(times,timeVol2_portion_0_6,'DisplayName','Target = 1.2
    m','Marker','^','MarkerSize',6,'MarkerIndices',1:5:length(times),'LineWidth',2)
semilogx(times,timeVol3_portion_0_6,'DisplayName','Target = 1.8
    m','Marker','|','MarkerSize',8,'MarkerIndices',1:5:length(times),'LineWidth',2)
semilogx(times,timeVol4_portion_0_6,'DisplayName','Target = 2.4
    m','Marker','v','MarkerSize',6,'MarkerIndices',1:5:length(times),'LineWidth',2)
semilogx(times,timeVol5_portion_0_6,'DisplayName','Target = 3.0
    m','Marker','.','MarkerSize',20,'MarkerIndices',1:5:length(times),'LineWidth', 2)
semilogx(times,timeVol6_portion_0_6,'DisplayName','Target = 3.6
    m','Marker','s','MarkerSize',8,'MarkerIndices',1:20:length(times),'LineWidth', 2)
semilogx(times,timeVol7_portion_0_6,'DisplayName','Target = 4.2
    m','Marker','*','MarkerSize',8,'MarkerIndices',1:10:length(times),'LineWidth', 2)
```

```
xlabel('Time [s]')
ylabel('$\frac{\Sigma V_p}{V_0}$','Interpreter','latex','FontSize',25)
legend('Location','southeast')
xlim([0 120])
figure(11)
semilogx(times,timeVol1_portion_1,'DisplayName','Target = 0.6
    m','LineWidth',2)
figtitle = ['Plots of Fraction of Expired Particle Volume vs. Time, Cough
    v_{peak} = ', num2str(v_peak), ' m/s, background wind speed of 1 m/s'];
title(figtitle)
hold on
grid on
semilogx(times,timeVol2_portion_1,'DisplayName','Target = 1.2
    m','Marker','^','MarkerSize',6,'MarkerIndices',1:5:length(times),'LineWidth',2)
semilogx(times,timeVol3_portion_1,'DisplayName','Target = 1.8
    m','Marker','|','MarkerSize',8,'MarkerIndices',1:5:length(times),'LineWidth',2)
semilogx(times,timeVol4_portion_1,'DisplayName','Target = 2.4
    m','Marker','v','MarkerSize',6,'MarkerIndices',1:5:length(times),'LineWidth',2)
semilogx(times,timeVol5_portion_1,'DisplayName','Target = 3.0
    m','Marker','.','MarkerSize',20,'MarkerIndices',1:5:length(times),'LineWidth', 2)
semilogx(times,timeVol6_portion_1,'DisplayName','Target = 3.6
    m','Marker','s','MarkerSize',8,'MarkerIndices',1:20:length(times),'LineWidth', 2)
semilogx(times,timeVol7_portion_1,'DisplayName','Target = 4.2
    m','Marker','*','MarkerSize',8,'MarkerIndices',1:10:length(times),'LineWidth', 2)
xlabel('Time [s]')
ylabel('$\frac{\Sigma V_p}{V_0}$','Interpreter','latex','FontSize',25)
legend('Location','southeast')
xlim([0 120])
```

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