PyREM: Implementing a Computational Model of Airborne Respiratory Droplet-based Virus Transmission

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Abstract

The transmission of the SARS-CoV-2 virus responsible for the ongoing COVID-19 pandemic has been predominantly attributed to the inhalation of infectious particulates exhaled by asymptomatic individuals. A single breath can release thousands of respiratory droplets containing water and SARS-CoV-2 viral RNA. The water immediately begins evaporating to form droplet nuclei small enough to be affected by air currents that can then spread these pathogens over a greater distance. The aim of this project is to implement a computational model to investigate how droplet size, proximity, and ambient conditions such as temperature and humidity affect the airborne respiratory droplet-based transmission of such a virus. Our work is adapted from Dr. Gavin Buxton's "Spreadsheet Model of COVID-19 Transmission," which simulates each breath as an expanding Gaussian Puff and incorporates evaporation, air currents, and drag. Unlike Buxton's spreadsheet model, which uses iterative coupled numerical calculations over constant-duration discrete-time steps to estimate exposure, our Python-based respiratory exchange model (PyREM) utilizes a functional programming paradigm along with numerical methods to solve for the roots of analytically-derived non-linear equations to decouple calculations of droplet diameter, velocity, and spatio-temporal concentration, and thereby more precisely quantify an individual's accumulated exposure over a given period of time. The results indicate that the viral exposure increases markedly as the distance from the infected source decreases and that heat and dryness contribute to higher exposure as well. Due to its modularity, PyREM can be easily extended to investigate other variables such as masks, turbulent airflow, and the presence of HVAC systems.

1. Introduction

With over forty mutated strains identified today, COVID-19 continues infecting individuals to varying degrees across the globe [1]. In the beginning, the exposure to contaminated surfaces and objects as well as direct contact with an infected individual was thought to be the main means of contracting the virus. However, the rampant growth in the infection rate suggested that there may be another mode of transmission responsible for the exponential spike in cases. Epidemiologists suggest that COVID-19 is primarily transmitted through indirect contact when an asymptomatic individual releases respiratory droplets into the air containing SARS-CoV-2 viral RNA [2]. These contaminated pathogens reside inside of respiratory droplets that are released every time a

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person coughs, sneezes, or even breaths [2]. A single breath can release thousands of respiratory droplets into the environment [3].

In this project, we are interested in modeling the behavior of intermediate size droplets that linger in the air for a short period of time before hitting the ground and contaminating surfaces. Our goal is to simulate how these intermediate droplets, which are neither considered aerosols nor large fomites, behave in order to quantify an individual's accumulated exposure to the virus. We will also more specifically analyze the impacts of proximity, temperature, humidity, and droplet size on the viral exposure.

Our work is adapted from Professor Gavin Buxton's "Spreadsheet Model of COVID-19 Transmission: Evaporation and Dispersion of Respiratory Droplets," [2] and is a python based implementation of the model described in that paper. Buxton's approach is a spreadsheet model that lies at the intersection of physics, mathematics, and computer simulations. The analytical models of his method can be broken down into three main aspects. The first is modeling the projectile motion of the respiratory droplets which incorporates drag force and terminal velocity. The second aspect is evaporation dynamics which include equations for droplet evaporation that determine the size of the diameter, ultimately, affecting the terminal velocity and lastly fluid dynamics that depend on the Reynolds number and surrounding air currents. Each breath is modeled as a Gaussian distribution of respiratory droplets or 'puff' that is expanding towards a healthy individual x meters away. Due to the limitations of a spreadsheet implementation, Buxton's model uses iterative coupled numerical calculations over constant-duration discrete-time steps to estimate the total exposure.

In this overview, we present how the design and architecture of our python-based respiratory exchange model (pyREM) is a computational implementation that more precisely quantifies the spatio-temporal concentration compared to the method used in the prior work [2]. It will also include the numerical results that we have generated as well as a brief description of how our current model can be extended to investigate other dependencies.

2. PyRem Design and Architecture

As illustrated in figure 1, our project is a sequence of functions that utilize a functional programming paradigm to simulate the evaporation, dispersion, and trajectories of the respiratory droplets. Given the required input parameters, pyREM computes the accumulated viral exposure through a series of decoupled function calls.

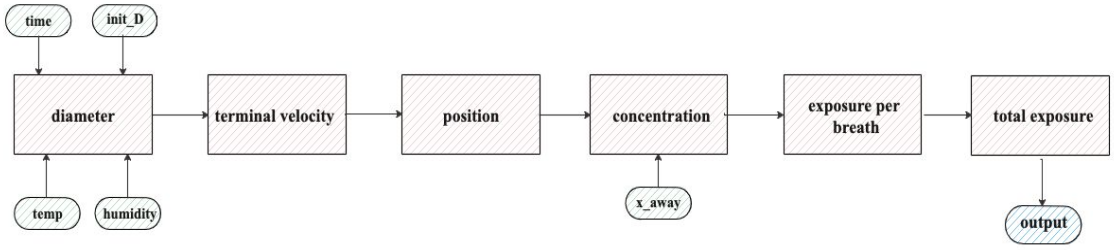

Figure 1: Block Diagram depicting the sequence of our program's execution that uses a functional programming paradigm.

From [2] (section 3b.) we could derive the following expressions for the diameter of the droplet in terms of D_0 the initial droplet size, D the molecular diffusivity of water vapor, P_{sat} and P_∞ the saturation of ambient water vapor pressure, t the time, R_v the specific gas constant for water, and ρ the density of water.

$$diameter\ polynomial:\ d^4 - Md^2 + K = 0 \qquad \textbf{(1)}$$

where, $M = D_0{}^2$ and $K = \frac{8D\,(P sat - P_\infty)\,t\,D_0{}^2}{\rho\,R_v\,T}$

We could also derive the following expression for the terminal velocity ([2] section 2a.) in terms of the parameters μ the viscosity of air, d the diameter of the droplet, g the gravitational acceleration, ρ_a the density of air and ρ_d the density of the droplet.

$$velocity\ exponential:\ Pv^{2.687} + Kv^2 - Nv = 0 \qquad \textbf{(2)}$$

where, $P = 10.8\mu\,(\frac{\rho_a\,d}{\mu})^{0.687}$ and $K = 72\mu$ and $N = 4d^2g\,(\rho_d - \rho_a)$

These non-linear equations for diameter and velocity could be solved to compute the corresponding values. We have derived these equations to decouple the numerical calculations and avoid the spreadsheet model's approach that estimates the diameter and velocity by using values of intermediary variables at previous iterations. Not only does this approach more precisely calculate these variables, but also enables us to set the smallest value of diameter to the last real root returned by the droplet polynomial instead of using a constant fraction from the spreadsheet model. We could also directly integrate the expression for concentration in the Gaussian puff model with respect to time rather than Buxton's approach of summing the values of concentration at each constant-duration time step.

3. Numerical Results

We present plots from our simulation that provide insight into both the intermediate quantities as well as how the concentration varies with different parameters.

3.1 Intermediate results:

We first present the results that visualize some of the intermediate quantities such as the diameter, vertical velocity, trajectories, and concentration.

Figure 2 illustrates how the diameter of the droplet varies with time for different initial droplet diameters. The physics model presented in [2] that we have used results in a different final diameter for each initial diameter, however, it does not appear to be the case that the minimum diameter is 44% of the original diameter as suggested by another reference [4, 5] cited in that paper. The lowest ratio of final to initial diameter observed in our experiments was ~71%. For values of D_0 below 23 microns, we found that the diameter does not change.

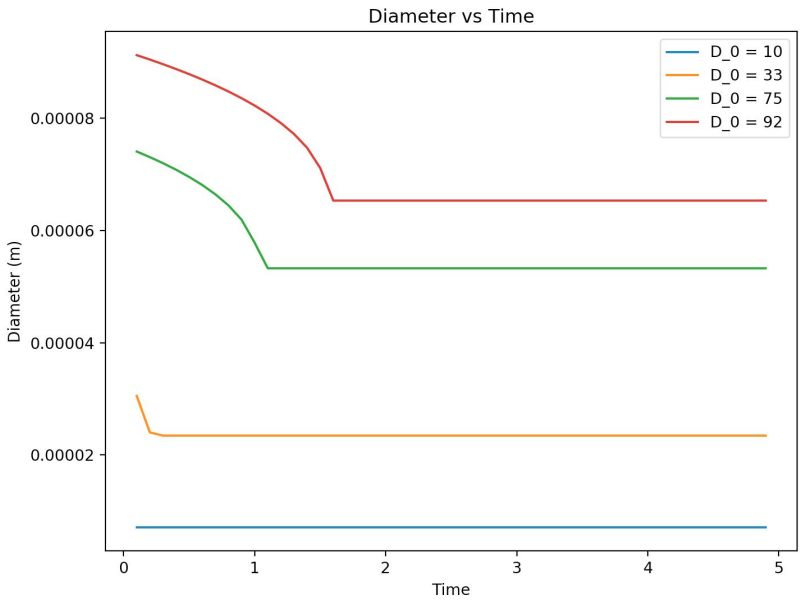

Figure 2: This plot illustrates the evaporating diameter of a respiratory droplet after 5 seconds for various initial droplet sizes.

Figure 3 shows how the vertical terminal velocity of the droplet varies with time for different initial droplet diameters. We see that the terminal velocity generally decreases up to a minimum value that is different for each initial diameter. Smaller droplets tend to start slower and not show a significant change in the terminal velocity from their initial velocity.

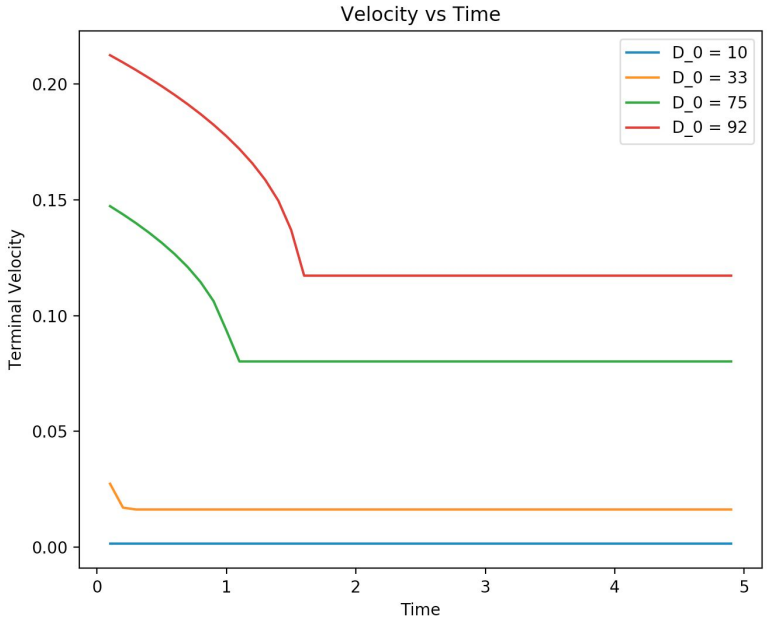

Figure 3: This plot illustrates the terminal velocity of the droplet with respect to time after 5 seconds for various initial droplet sizes.

Figure 4 shows how the horizontal position of the droplet varies with time - this is just a straight line with a constant slope reflecting the constant air current velocity of 1m/s.

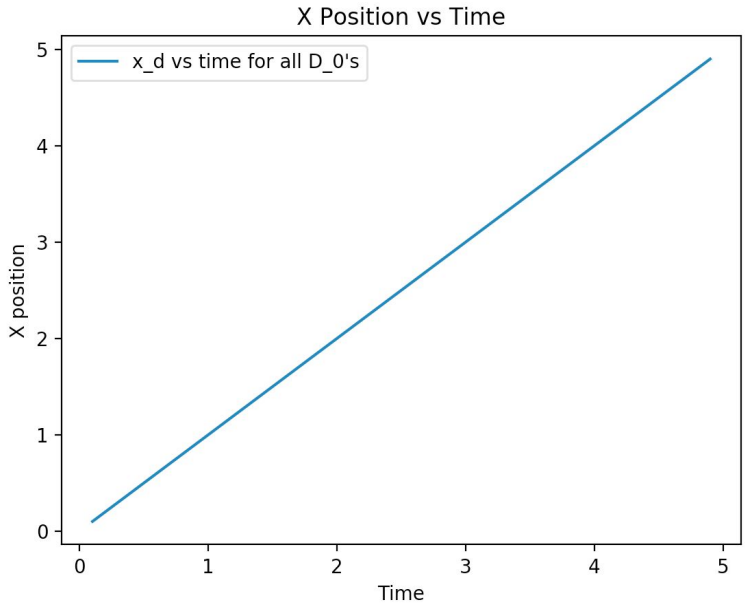

Figure 4: This plot illustrates the horizontal position of the droplet with respect to time after 5 seconds for all initial droplet sizes.

Figure 5 shows how the vertical position of the droplet varies with time for different initial droplet diameters. Due to their high terminal velocities, larger droplets experience a greater change in their vertical position compared to smaller droplets that can linger in the air for longer periods of time and also be carried away by wind velocities.

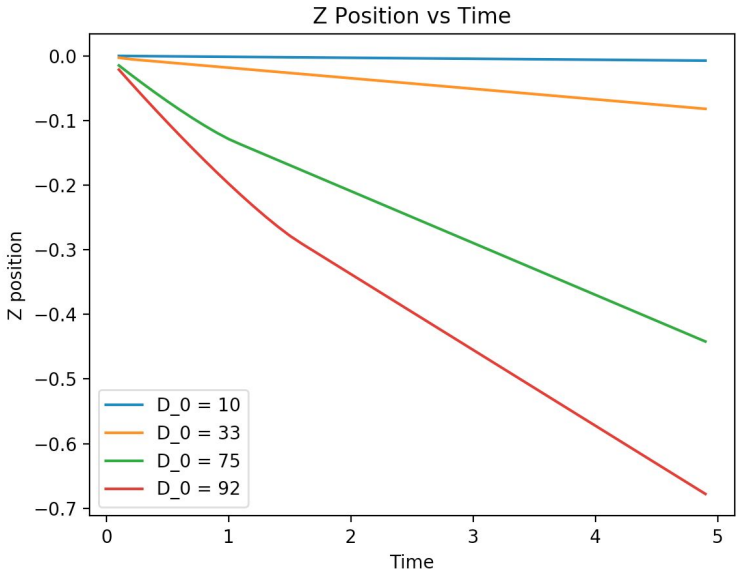

Figure 5: This plot illustrates the vertical position of the droplet with respect to time after 5 seconds for various initial droplet sizes.

Similarly, Figure 6 illustrates the trajectory of each droplet by plotting the horizontal vs vertical position for different initial diameters.

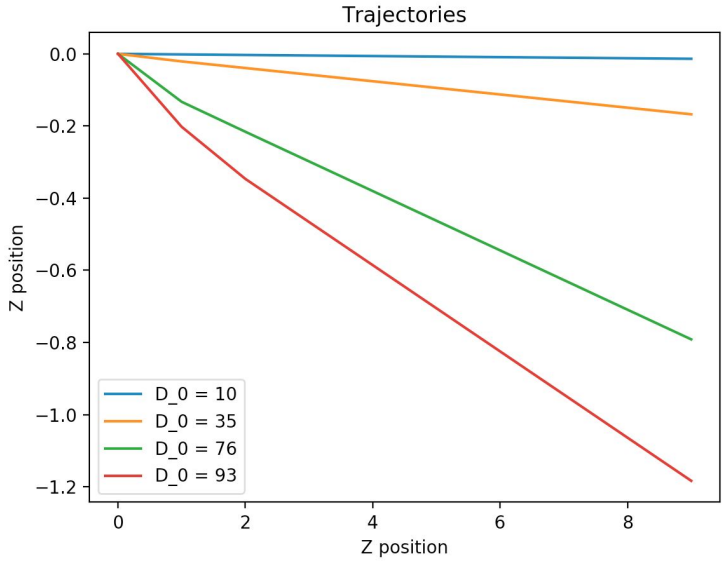

Figure 6: This plot illustrates the vertical position vs horizontal position of the droplet after 10 seconds for various initial droplet sizes.

In Figure 7 we plot the concentration function from the Gaussian puff model with respect to time for different initial diameters. As illustrated in the plot, the concentration of the puff after 5 seconds is significantly greater for smaller droplets compared to larger ones. This reiterates that small respiratory droplets have a greater impact on spreading the virus by lingering in the air compared to large fomites that infect surfaces and objects [2].

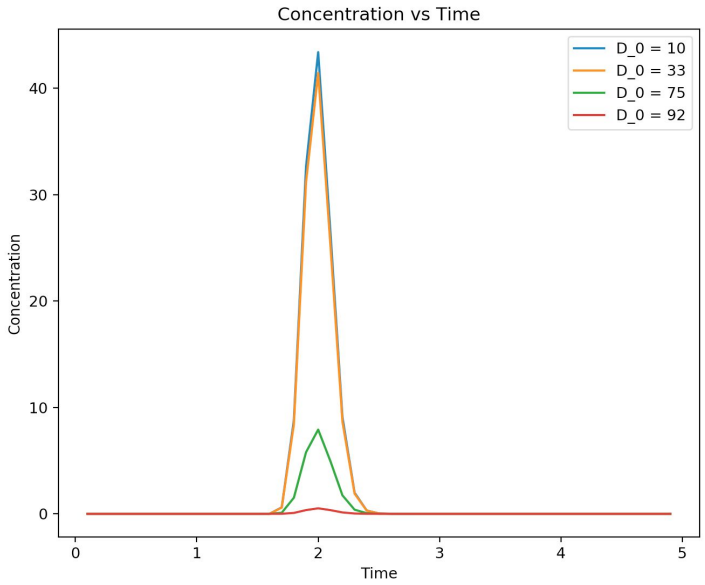

Figure 7: This plot shows the curves of the concentration function vs time for various initial droplet sizes at 5 seconds.

3.2 Replicated results:

The following figures all match quite closely the corresponding figures generated in [2]. In order to compare the numerical results of pyREM to Buxton's model that plots the dose of the droplets relative to the dose of smaller droplets, we have normalized our curves using the value of concentration for a 1-micron droplet at the default input parameter values.

Figure 8 plots the viral concentration of respiratory droplets as a function of droplet size for different relative humidities. This plot depicts the inverse relationship between concentration and humidity since greater levels of moisture decrease the evaporation rate which leads to larger terminal velocities causing the droplets to more quickly fall to the ground.

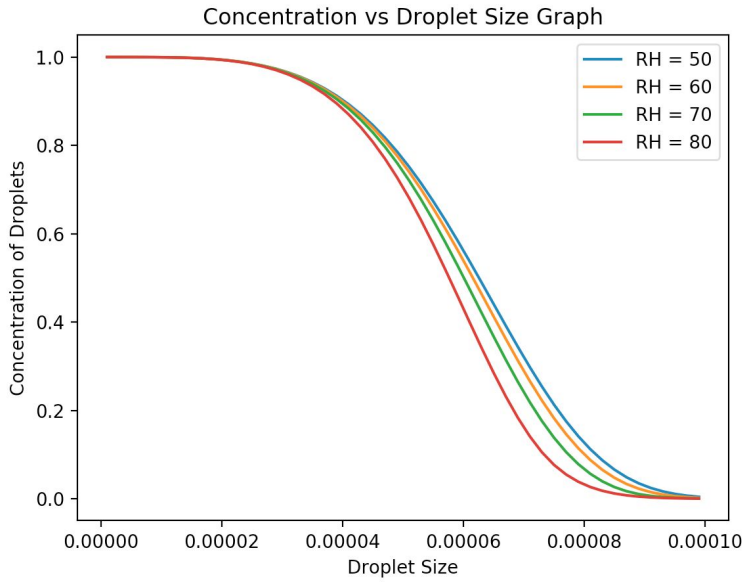

Figure 8: Illustration of how relative humidity affects the accumulated concentration of droplets approaching an individual 2 meters away as a function of the droplet's initial size.

Figure 9 shows the direct relationship between concentration and temperature by again plotting the concentration as a function of droplet size for several temperature values. In this case, the accumulated viral exposure is greater in high-temperature environments because the heat catalyzes the evaporation rate causing larger droplets to aerosolize and be transmitted through airflow.

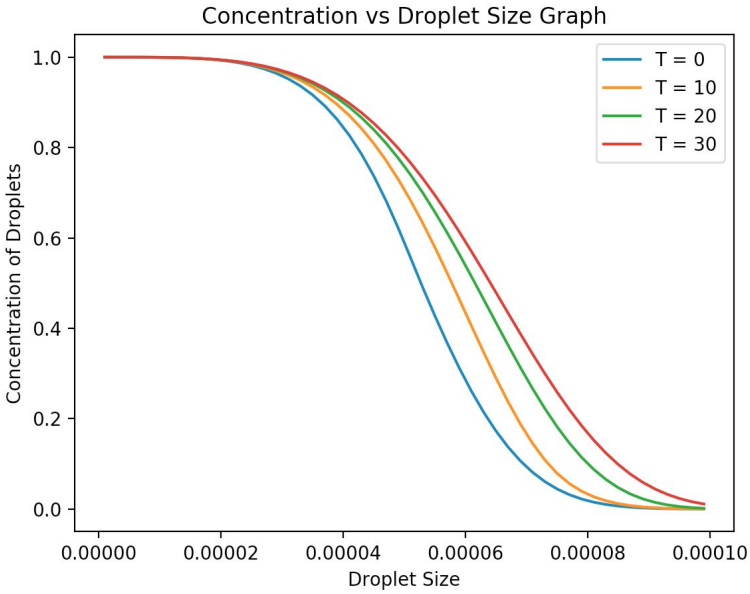

Figure 9: Illustration of how ambient temperature in Celsius affects the accumulated concentration of droplets approaching an individual 2 meters away as a function of the droplet's initial size.

Our last plot, figure 10, is perhaps the most significant figure out of all the results because it shows the effects of social distancing on the respiratory droplet-based transmission of COVID-19 by varying the separation distance. Similar to the previous figures, the concentration is plotted as a function of droplet size for various x_away values. The plot shows that the viral exposure markedly increases as an individual is closer to an infected source.

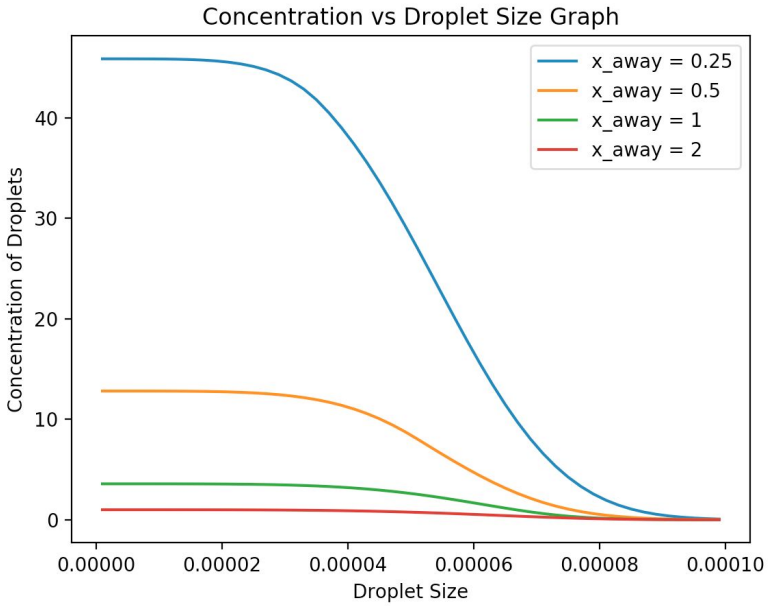

Figure 10: Illustration of how proximity affects the accumulated concentration of droplets approaching an individual x meters away as a function of the droplet's initial size.

4. Summary and Conclusions

As we have shown, our PyREM implementation matches the results from Buxton's spreadsheet model in [2]. The code of our implementation is made available as an open-source at https://github.com/ANRGUSC/pyREM.git. The modular design we have followed can easily accommodate extensions and modifications to investigate the effects of masks, turbulent airflow, and the presence of HVAC systems on an individual's accumulated exposure over a given period of time.

References

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[2] Buxton, Gavin. Spreadsheet Model of COVID-19 Transmission: Evaporation and Dispersion of Respiratory Droplets, Spreadsheets in Education, vol 12, no. 2, May 2020. Available online at: https://sie.scholasticahq.com/article/12861-spreadsheet-model-of-covid-19-transmission-evaporation-and-dispersion-of-respiratory-droplets

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[4] Siobhan K Halloran, Anthony S Wexler, and William D Ristenpart. A comprehensive breath plume model for disease transmission via expiratory aerosols. PloS one, 7(5), 2012**.**

[5] Mark Nicas, William W Nazaroff, and Alan Hubbard. Toward understanding the risk of secondary airborne infection: emission of respirable pathogens. Journal of occupational and environmental hygiene, 2(3):143–154, 2005.