Modeling the infectiousness of droplets when exposed to ultra-violet germicidal system: A computational fluid dynamics approach

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Abstract. Corona viruses rapidly spread in humans and vertebrates, cause respiratory, enteric, hepatic, and neurological diseases. Due to the risk associated with corona viruses, many studies have attempted to identify mitigation measures to reduce its infectiousness and understand its dynamics, evolution and control. Despite the progresses, there is limited modelling data that shows the decay process of the corona virus infectiousness in a confined environment, when subjected to ultra-violet germicidal irradiation (UVGI) system. Hence, in this study we report the result of a mathematical model that predicts the infectiousness of corona virus while evolving using computational fluid dynamics. A prototype of a UV system was constructed as a fluid domain filled with air. The droplets were modelled using the discrete phase approach under transient flow conditions. Droplets particles were injected from the inlet at 5 ms^{-1} to a fluid domain and allowed to move in the ambient flow, subject to illumination with UVGI in the regions of the fluid domain. The survival rate of the droplet follows an exponential decay as the concentration reduces. The results of this study show that our modelling describes the viral concentration,and its reduction over time, in the droplet for different scenarios. The model can be used to predict infectiousness of the droplets when subjected to a UVGI system in these different scenarios. Ultimately, the model will be used to inform and optimise the design of engineered interventions.

1. Introduction

Coronavirus disease 2019 (COVID-19) is an infectious disease that was declared a pandemic in 2020 [1, 2] due to its high level of transmissibility and spread across different continents. COVID-19 is caused by a novel betacoronavirus, which is named severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). COVID-19 with small droplets are aerosols which

could be classified as one of the main sources of air pollutants in a confirmed environment [3]. Furthermore, the coronavirus as an infectious disease is mainly inhaled as droplets from carriers and patients [4, 5].

Studies focusing on finding solutions to mitigate the spread and dangers associated with the viruses in human health have been going on since the discovery of the COVID-19 disease [6]. Amongst those studies are reports that are generally based on experimental and theoretical methods [7]. The main transmission mode of COVID-19 is human to human via propagation in the form of droplets and close contact.

The studies of the evolution and spread of the COVID-19 using computational fluid dynamic approach (CFD), other numerical approaches and experimental techniques have been chronicled [7]. CFD is an approach that can be used to model the physical behaviour and evolution of fluids and droplets [8] and the transmission of airborne infectious diseases.

People in a confined place such as an aircraft, commuter buses and hospitals are likely to be highly susceptible to airborne contagious agents [9]. Reports suggesting a higher risk of infectious disease transmission in confined environments, in particular those environments with poor ventilation have been reported [10, 11]. The CFD method has been used to validate COVID-19 infection data in confined environments, for example, a train as in [12]. The formation of droplets of saliva has been numerically modelled using the CFD. An example is the report on the droplets from the mouth and lips of an infected person during the sneezing process [13]. From this point on, the COVID-19 transport could be modelled as propagating droplets [13]

The ultra-violet germicidal irradiation (UVGI) system is a technique employed to deactivate the potency of viruses, and has been used to reduce the survival rates of infectiousness in an open place [14]. Studies are carried out through the simulation of the transport of respiratory aerosols within a specific fluid domain. The combination of the CFD and the UVGI system is essential as the technicalities and inherent characteristics of the combined process could help to introduce an enhanced technology which could assist to understand and mitigate the survival rate, the propagation and evolution of droplets [15, 14]. Despite the numerous studies that reported the spread and control of COVID-19, there are still more to be understood. For instance, the survival rate of the COVID-19 when exposed to the UVGI system in confined environments such as ambulances, taxis and hospitals are not yet fully understood. It is imperative that the evolution and spread of the COVID-19 in confined environments should be well understood to mitigate the transmission of diseases and virsues.

In this study, we present a CFD model of the evolution of the infectiousness of a droplet in a confined environment when subjected to a UVGI system. The CFD as implemented in ANSYS Fluent (v2020R2) was used to model the survival rate of droplets in a confined environment as the droplets moved through the UVGI system. Additional code, which was used to model the effect of the UVGI on the viruses within the droplets, was developed and added to the CFD model. We adopted the discrete phase model (DPM) with specific boundary conditions as listed in Table 1 for the simulations. We show that the infectiousness of the droplets reduced as the droplets pass through the UVGI system. The results of this study is envisaged to be implemented for the study of the control and spread of infectious diseases such as corona viruses and tuberculosis. A companion study in this same proceedings assesses the attenuation of the infectiousness due to droplet evaporation, and these two approaches are designed to be combined in a subsequent study.

2. Methodology

Viruses spread in the air is assumed to flow in small droplets. The Navier-Stokes equation for viscous incompressible flow employed to describe the air flow as experienced by droplets during propagation. The Navier-Stokes (governing equations) for airflow given as:

$$\frac{\partial u_i}{\partial x_i} = 0, \quad \frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_i} = -\frac{1}{\rho}\left((v + v_T)[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}] \right), \tag{1}$$

where m, u, T, v, are mass, velocity, turbulence and viscosity, respectively. The i, j = 1, 2, 3 are the components of the velocity vector and the spatial coordinates. Turbulence is modelled using the standard $k - \epsilon$ model.

The CFD approach as implemented in the ANSYS Fluent (v2020R2) and employing the discrete phase model (DPM) were used for the modelling of the infectiousness of droplet passing through a UVGI system. When using the DPM to model the flow of a droplet, the trajectories can be determined by integrating the force balance in the Lagrangian reference frame. The particle inertial as well as the forces acting on the droplet should be equal to the force balance in the Lagrangian frame given in:

$$m_p \frac{d\mathbf{u}_p}{dt} = m_p \frac{18\mu}{\rho_p d_p^2} \frac{C_D Re}{24}(\mathbf{u} - \mathbf{u}_p) + m_p \frac{\mathbf{g}(\rho_p - \rho)}{\rho_p} + m_p \frac{\rho}{\rho_p} \mathbf{u}_p \nabla \mathbf{u} + \bar{F}_{other} \tag{2}$$

A UVGI test-system was constructed as a rectangular box with $500 \times 160 \times 60$ mm dimension, placed in a relatively confined room. The performance of a typical UVGI depends on airflow patterns, air velocity amd lamp position. Hence, the rectangular fluid domain is filled with air with its meshing scheme as shown in Figure 1. The energy equation and k-epsilon viscous model were used. Acceleration due to gravity was set to 9.82 ms^{-2}. In the DPM, the integration with continuous phase was used to describe the droplet transition through the fluid domain. The infectiousness was described by a scalar parameter associated with each droplet. The scalar was updated via a user defined function (UDF) which described the survival rate. The Rorim-Ramler diameter distribution was use to describe the ensemble of droplet diameters. In the particular example, the droplets maximum(minimum) and number of diameters were $10^{-4}(10^{-8})$ m and 100, respectively. Droplets were injected from the emission region using the face normal direction as shown in Figure 1. The injection and inlet velocities were set to 5ms^{-1} and the turbulence intensity and viscosity ratio for both the inlet and outlet were set to 5 and 10 respectively. The outlet pressure was set to Zero. The discrete phase boundary conditions for the inlet and outlet were set to escape whereas the stationary wall was set to trap with no slip condition allowing droplet to get trapped when they come in contact with the wall. Additional details of the computations parameters are shown in Table 1.

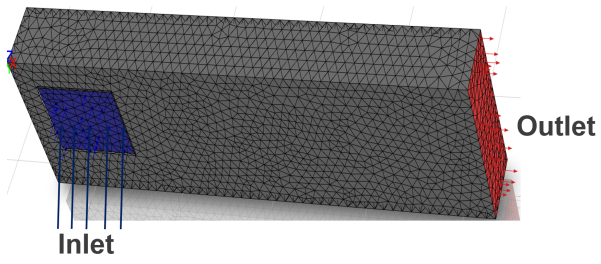

Figure 1: A rectangular box with $500 \times 160 \times 60$ mm dimension showing the inlet and outlet boundary conditions of the fluid domain.

The simplest case of a droplet containing microorganisms are treated as simple object with parameters such as mass, momentum and energy. The UV dose $D(r,t)$ is defined as the product of the irradiance $I(r,t)$ and exposure time t. The irradiance $I(r,t)$ (Wm^{-2}) is a function of time and position $r(x,y,z)$, where the x, y, and z are the position coordinates.

Table 1: Input parameters and boundary conditions imposed for the modeling of droplets

Quantity	Description
Model	Discrete phases
Diameter of particles	$1-4$ μm
Material taken	water-liquid
Temperature of particles	25°C
Flow rate	2.51×10^{-7} Kgm^{-3}

The position of a droplet with respect to the $I(r,t)$ at a point source is defined as $r(x,y,z) = \sqrt{(x_1-x_2)^2+(y_1-y_2)^2+(z_1-z_2)^2}$.

The survival rate (S_R) of microorganisms passing through the UVGI system is defined as

$$S_{\mathrm{R}} = \frac{C_t}{C_0}\exp^{-KIt} \tag{3}$$

where C_t, C_0, K, I and t are the microorganism concentration level after exposure for t seconds, the initial concentration of the microorganism from the inlet, the UV sterilization coefficient (m^2J^{-1}), the irradiance and time, respectively. While the concentration $C(r,t)$ is a function of space and time, the K is a characteristics of how each microorganisms is sensitive to the UVGI system. The sterilization effect of the UVGI system are mostly determined by the K, I and t. The survival rate in Equation 3 can be written in its differential form as

$$\frac{\partial C}{\partial t} = -\mathrm{KIC}, \tag{4}$$

where C is the concentration of microorganism per unit volume within the droplet. Equation 4 enables us to calculate the concentration time evolution of airborne microorganisms decreased in small steps by a UVGI system. The value of K for any microorganism is determined experimentally in separate studies.

3. Results and Discussion

In this study, we have considered the droplets UVGI scenarios in four different conditions (case I, case II, case III and case IV) as they passed through the fluid domain. In all conditions, we placed the UVGI system in a confined environment where the pathogen carrying aerosols are instantaneously and uniformly distributed.

For the first simplest condition (case I), C_0 the initial concentration of virus within the droplet and I the irradiance are fixed to be the same for all source positions as the droplets move from one cell to the other. The plot of the resulting droplet infectiousness concentration is shown in Figure 2. All droplets started from the same initial concentration point with a decreasing exponential decay with the same slope (due to the same irradiance). The above shows in the first simple context that he scalar tracking of the droplet was reduced as expected when subjected to the UVGI system. The log-linear plot shown in Figure 2 for the time dependent droplet viral concentration are in the same straight line with the survival rate obeying an exponential decay as expected with the assumptions.

For the second condition the initial viral concentrations of droplets were still assumed to be constant. That is all the droplets have the same infectiousness at the inlet, however, the irradiance is now varied as the droplet passes through the fluid domain. The irradiance is set to be inversely proportional to the square of the distance apart of the droplets from the irradiation (point) source ($I \propto 1/r^2$). Hence, the irradiance term in Equation 4 could be expressed as $I = \kappa/r^2$; where κ is the constant of proportionality. For simplicity, we assumed κ to be unity.

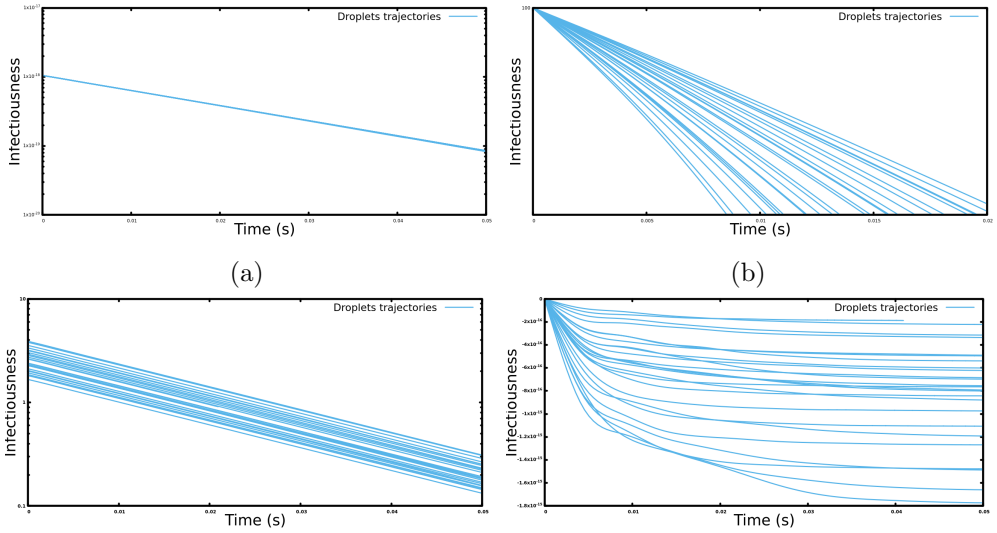

Figure 2: The log-linear plots of the survival rate of droplets (a) as a function of uniform fixed irradiance, uniform initial viral concentration and time, (b) when the irradiance is varied proportional to the inverse square of the droplet-point source distance (c) when the initial viral concentration is varied with the initial position of the droplets in the UVGI system and (d) when the irradiance is a function of the position of the droplets as in (b) and the droplets move substantially through the UVGI system, sampling a larger variation of irradiance values

At this stage, the value of κ and the functional form of the $I(r.t)$ is arbitrary, but it can later be determined from measurement or modelling. Base on case II, the Equation 4 can now be written as

$$\frac{\partial C}{\partial t} = -\mathrm{KC}\frac{\kappa}{\mathrm{r}^2}. \tag{5}$$

The droplets behavior with respect to Equation 5 is shown in Figure. 2b. The results confirm that the droplet viral concentrations obey the exponential decay law with a range of almost constant infectiousness due to the variation of the irradiance.

In the case III, the droplets were assumed to experienced uniform irradiance. However, the initial infectiousness of the droplets which is proportional to the initial droplet volume ($C \propto V_\vartheta$) changes. The initial volume (V_ϑ) is defined as the m/ρ_ι, where m is the mass of the droplet and the ρ_ι is the density. Hence, case III concentration is mathematically equivalent to $C_0 = \eta \times (m/\rho_\iota)$. Therefore, applying the the assumption of case III into Equation 4 will yield

$$\frac{\partial C}{\partial t} = -\mathrm{KI}\eta\frac{m}{\rho_\iota} \tag{6}$$

The plot of the droplet survival rate in response to the concentration and irradiance is shown in Figure 2c. The droplets have different viral concentrations at the inlet, however, they all are exposed to the same irradiance throughout their life span in the UVGI system. For case III, the droplets maintained the same slope in the log-linear plot as expected all through the UVGI system. Finally, the droplets are considered to have the same initial viral concentration. However, they experience non uniform irradiance which also evolves as they travel through the fluid domain for the case IV condition. In this category, Equation. 4 is represented as

$$\frac{\partial C}{\partial t} = -\mathrm{K}\eta\frac{m}{\rho_\iota}\frac{\kappa}{r^2}. \tag{7}$$

As shown in Figure 2d, the droplets spread across with different and changing slopes. This is due to the different irradiance as they are transported from one cell to the another in the fluid domain. In the general case, the droplets should be modeled to experience different irradiance as a function of position, different initial volumes and finally, when coupled to the evaporation model with time evolving volume. The model shows that the exponential decay of the survival rate depicts the reduction in the life spna, potency and efficacy of the transported microogranisms

4. Summary

The results of the modeling of the time evolving infectiousness of droplets moving through a UVGI system in a confined environment were reported. By using the computational fluid dynamics approach, the behavior of the droplets in the UVGI system as subjected to four different conditions were ascertained. The survival rate of the droplets and their infectiousness exhibit an exponential decay behaviour. The droplets concentration reduced as they pass through the UVGI system. Four conditions were selected to exhibit separately different simple exponential behaviour as the droplets are transported in the UVGI system as expected in the simple case. These results show that the effect of the UVGI can be accommodated within the CFD simulation by the method of additional code deployed as a User Defined Function to describe the scalar property of time evolving infectiousness for each droplet. In addition, the evaporation model of the companion paper will be accommodated in the same CFD model in the future.

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Reference

[1] Di Gennaro F, Pizzol D, Marotta C, Antunes M, Racalbuto V, Veronese N and Smith L 2020 *International journal of environmental research and public health* **17** 2690
[2] Bhimraj A, Morgan R L, Shumaker A H, Lavergne V, Baden L, Cheng V C C, Edwards K M, Gandhi R, Muller W J, O'Horo J C *et al.* 2020 *Clinical Infectious Diseases*
[3] He Q, Niu J, Gao N, Zhu T and Wu J 2011 *Building and Environment* **46** 397–408
[4] Ai Z, Mak C M, Gao N and Niu J 2020 *Building Simulation* vol 13 (Springer) pp 489–496
[5] Giovanni A, Radulesco T, Bouchet G, Mattei A, Révis J, Bogdanski E and Michel J 2021 *European Archives of Oto-Rhino-Laryngology* **278** 1687–1692
[6] Ashby M P 2020 *Crime Science* **9** 1–16
[7] Khan S, Siddique R, Ali A, Xue M and Nabi G 2020 *Journal of Hospital Infection* **104** 449–450
[8] Messa G V, Yang Q, Adedeji O E, Chára Z, Duarte C A R, Matoušek V, Rasteiro M G, Sanders R S, Silva R C and de Souza F J 2021 *Processes* **9** 1566
[9] Sodiq A, Khan M A, Naas M and Amhamed A 2021 *Environmental Research* **199** 111329
[10] Dbouk T and Drikakis D 2021 *Physics of Fluids* **33** 011905
[11] Hu M, Lin H, Wang J, Xu C, Tatem A J, Meng B, Zhang X, Liu Y, Wang P, Wu G *et al.* 2021 *Clinical Infectious Diseases* **72** 604–610
[12] Wang Z, Galea E R, Grandison A, Ewer J and Jia F 2022 *Safety science* **147** 105572
[13] Mesgarpour M, Abad J M N, Alizadeh R, Wongwises S, Doranehgard M H, Ghaderi S and Karimi N 2021 *Journal of Hazardous Materials* **413** 125358
[14] Buchan A G, Yang L and Atkinson K D 2020 *Scientific reports* **10** 1–7
[15] Kanaan M 2019 *Case Studies in Thermal Engineering* **15** 100535