

Research Article

Numerical Modeling and Simulation of the Droplet Transmission of SARS-CoV-2 in the Ambient Environment and Its Relevance to Social Distancing

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In SARS and influenza-type infections, the transmission of the viral particles from the infected individual to the susceptible individual involves the respiratory route. The current novel CoV2 transmission also involves a similar mechanism. The virus particles are present as droplets ranging from 5 to 10 μm in diameter and are expelled into ambient air when the infected individual coughs, sneezes, or even speaks. These tiny droplets move over a distance through the atmosphere, and the initial velocity determines the maximum distance the droplets reach. In this work, a computational fluid dynamic model was developed using Ansys Fluent software, incorporating the physical characteristics of the viral droplets and the ambient atmosphere. The movement of these particles was analyzed for three different initial velocities of 1, 5, and 10 m/s. Furthermore, the maximum distance traveled by the simulated particles for higher velocities was analyzed using a linear regression model. Results demonstrate that the simulated viral particles embedded in the droplets can travel a maximum distance of 1.24 m for an initial velocity of 10 m/s. Furthermore, an increase in the initial velocity to a value of 30 m/s results in the particle's movement to a maximum distance of 2.595 m. The study results indicate that at least 2.5 meters distance has to be maintained for effective social distancing to prevent the further spread of the novel CoV2 transmission. Even after the lifting of the lockdown, institutional social distancing needs to be practiced to abate the transmission to a near-zero level and to prevent a rebound. In public places such as public transport and shopping malls, strict adherence to wearing masks must be made mandatory by social regulation.

1. Introduction

The transmission of respiratory viral infections involves several factors such as generation and dispersion of the expiratory droplets, the infectivity of the pathogens, survival on surfaces, environmental factors, and deposition of droplets in susceptible contacts [1]. From 1918 to 1920, the Spanish flu resulted in more than 500 million infections worldwide and 17 to 50 million deaths [2]. Furthermore, the SARS epidemic from 2002 to 2003 resulted in 8,098 cases

and 774 deaths. The swine flu pandemic during 2009-2010 affected 213 countries and caused more than 16 thousand deaths. Furthermore, since September 2012, there has been a reported 858 MERS-CoV-related deaths [3].

The most common transmission modes of the flu and flu-like respiratory infections are droplets airborne or direct contact with the infective respiratory secretions expelled by the infected persons [4]. The transmission by direct contact is established by inhalation of the virus aerosols by the contact receptors at a short distance [5]. However, if such

airborne transmission of the viral infections is unrecognized in the initial stages, it leads to the onset of the epidemics [6]. Humans can discharge aerosols in different actions such as coughing, sneezing, and speaking [7]. Respiratory infectious diseases are transmitted to non-infected people through droplets and particles of different sizes. Dugid observed a significant proportion of the droplets in 4 to 8 and 8 to 16 microns in coughing and sneezing [8]. The transmission of infectious diseases requires a few other components, such as the surrounding environment, the concentration of infectious droplets, ventilation, the exposure time, and the immune defense mechanism of the exposed individual [9].

Recent studies indicate that the H1N1 virus can be transmitted when the infected individual sprays droplets of different sizes to the surrounding environment during coughing and sneezing. While the smaller droplets $<2.5 \mu$ get dried up and suspended in air, the large droplets get settled on the surfaces [10]. When the dried droplets are re-suspended in the environment, the re-suspended particles can remain airborne for prolonged durations, as seen in influenza epidemics [11]. The infectious airborne droplets are also responsible for tuberculosis transmission. Furthermore, an infected person expels infective particles while speaking. Within five minutes, he or she expels many infectious droplets similar to one bout of cough, and these droplets remain suspended in the environment for 30 minutes [3].

Contagious viruses are usually carried by droplets expelled through sneezing and coughing. These droplets spread to the ambient surroundings, making them highly contagious. Therefore, it is essential to know the maximum distance traveled by such droplets to prevent the spread of the infection from one person to another and to establish proper social distancing protocols during outbreaks of the flu and flu-like epidemics, including the current novel CoV2 pandemic. It has been shown that the evaporation of the water droplets less than $100 \mu\text{m}$ takes place in milliseconds, and the evaporation rate depends on the ambient air temperature and humidity. However, the evaporated particle residues get re-suspended in the atmosphere for a prolonged period.

On the other hand, the large droplets fall on the surface and remain infective depending on the surface to which the droplets adhere [7]. The size of the SARS-CoV-2 varies between 60–140 nm, and the infected persons expel many infective virus particles in each droplet after each cough, sneezing, and speaking. In this work, numerical analysis was carried out to determine the total distance traveled by a droplet containing the virus in response to various wind velocities. We considered $10 \mu\text{m}$ size droplets as the particles in the range of 8 to $16 \mu\text{m}$ are expected to be expelled in large numbers, especially during speaking. Droplets of 10 to $20 \mu\text{m}$ can carry 70 to 340 SARS-CoV-2 virus particles, and therefore they play a significant role in airborne transmission.

In recent years, several research works have been carried out to analyze the aerosolization of the droplets using high-precision computational fluid dynamics (CFD) approaches [12–14]. The CFD approach can provide an improved insight into complex distribution patterns of droplets. In the past,

the CFD approaches have been utilized to predict droplet transmission from humans in various environments such as an aircraft cabin, conference room, elevators, etc. [15]. Since the COVID-19 outbreak, researchers have focused on the CFD-based investigations on SARS-CoV-2 transmission from affected individuals through droplets. Bhatia and De Santis [16] used the $k-\omega$ ST turbulence model simulated using Ansys Fluent software to analyze the airborne SARS-CoV-2 dispersion in airplane cabins. The authors demonstrated a 75% chance of droplet transmission up to 2 m within the airplane cabin area. Shao et al. [17] used OpenFOAM software to analyze airborne SARS-CoV-2 transmission with or without ventilation in different scenarios. The authors concluded that ventilation helps decrease the quantity of contaminated air, but it may have a massive chance of increasing the spread of the virus into larger spaces.

In this work, a computational fluid dynamics approach performed in Ansys Fluent platform is utilized to analyze the droplet transmission from the SARS-CoV-2 affected individuals.

2. Materials and Methods

A sneeze or cough of a human being contains air, and the droplets of various sizes carry several organisms, including viruses which travel in the air. The distance traveled depends on the wind speed and the initial velocity of the sneeze or cough. In this work, a computer model was developed and tested to analyze droplet velocities. In the developed model, two phases were considered: the continuous phase (air) and the discrete phase (viral droplets). In order to determine the distance traveled by the viral droplet in the ambient environment, the continuous phase (air) was first simulated until a steady-state solution was obtained. After reaching a converged solution, the simulated droplets were injected using the “discrete phase method” in Ansys Fluent software. The initial velocity of the sneeze can vary from person to person, depending on their lung capacity and gravity. It has been shown by particle image velocimetry (PIV) that the velocity of cough varies between 1.5 m/s and 28.8 m/s [18]. The simulation of the developed model was carried out for three different forcing velocities, and a linear regression model was utilized to estimate the total distances traveled by the particles for higher initial velocities.

In the developed model, the diameter of the viral droplets was considered to be $10 \mu\text{m}$, and the initial velocities of 1 m/s, 5 m/s, and 10 m/s were employed for the simulation. The density of the droplets was set to 1000 kg/m^3 . A 2D rectangular computational domain was created with the size of $5 \text{ m} \times 1.5 \text{ m}$, and the inlet diameter was set to a value of 30 mm. The mesh adopted for this study is a structured mesh with quadrilateral elements, each of size equal to $10 \text{ mm} \times 10 \text{ mm}$. Furthermore, a total of 51000 mesh elements were employed to develop the model. Also, a domain independence study and grid independence study were carried out before adopting the above values. Figure 1 shows the computational domain considered for this analysis.

The Lagrangian discrete phase model that follows the Euler–Lagrange approach is used for the numerical

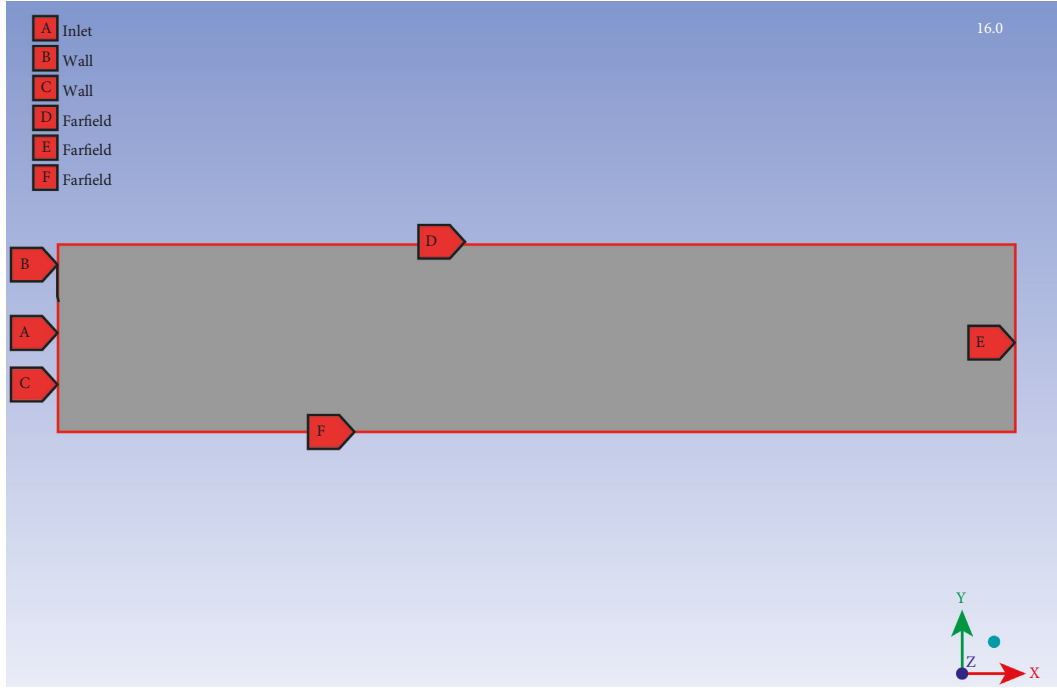


FIGURE 1: The developed computational domain has an inlet (A) of 30mm diameter comparable to a mouth, B and C as borders. D-E-F with a $1.5\text{ m} \times 5\text{ m}$ domain containing 51000 mesh elements is comparable to the ambient condition. Ansys Simulation tool provides far-field boundary conditions which can be used to denote an infinite region using a closed domain.

calculation. The fluid phase is treated as a continuum and solved using the Spalart–Allmaras turbulence model, while the dispersed phase is solved by tracking droplets through the calculated flow field. The dispersed phase can exchange momentum, mass, and energy with the fluid phase.

The trajectory of a discrete phase droplet is predicted by integrating the force balance on the droplet, which is written in a Lagrangian reference frame. This force balance equation is given as

$$\frac{du_p}{dt} = F_D(u - u_p) + \frac{g_x(\rho_p - \rho)}{\rho_p} + F_x, \quad (1)$$

where F_x is an additional acceleration (force/unit droplet mass) term, $F_D(u - u_p)$ is the drag force per unit droplet mass, and

$$F_D = \frac{18\mu}{\rho_p d_p^2} \frac{C_D \Re}{24}, \quad (2)$$

where u is the fluid phase velocity, u_p is the droplet velocity, μ is the molecular viscosity of the fluid, ρ is the fluid density, ρ_p is the density of the droplet, and d_p is the droplet diameter. \Re is the relative Reynolds number, which is defined as

$$\Re \equiv \frac{\rho d_p |u_p - u|}{\mu}. \quad (3)$$

The transport equation for eddy viscosity as solved by the Spalart–Allmaras model is given as

$$\rho u_i \frac{\partial \mu_t}{\partial x_i} = \frac{1}{\sigma_{\mu_t}} \left[\frac{\partial}{\partial x_j} (\mu + \rho \mu_t) \frac{\partial \mu_t}{\partial x_j} + C_{b\rho} \rho \left(\frac{\partial \mu_t}{\partial x_j} \right)^2 \right] + P_{\mu_t}, \quad (4)$$

where μ_t is the eddy viscosity and P_{μ_t} is the production term of turbulent viscosity. The values of constant terms are $\sigma_{\mu_t} = 2/3$ and $C_{b\rho} = 0.622$.

The conservation equations for laminar flow in an inertial (non-accelerating) reference frame are presented below.

The mass conservation equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = S_m. \quad (5)$$

(5) is the general form of the mass conservation equation and is valid for incompressible as well as compressible flows. The source S_m is the mass added to the continuous phase from the dispersed second phase (e.g., due to vaporization of liquid droplets).

Momentum conservation equations:

$$\frac{\partial}{\partial t} (\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot (\bar{\bar{\tau}}) + \rho \vec{g} + \vec{F}, \quad (6)$$

where p is the static pressure, $(\bar{\bar{\tau}})$ is the stress tensor (described below), and $\rho \vec{g}$ and \vec{F} are the gravitational body force and external body forces (e.g., that arise from interaction with the dispersed phase), respectively.

The stress tensor $(\bar{\bar{\tau}})$ is given by

$$(\bar{\bar{\tau}}) = \mu \left[\left(\nabla \vec{v} + \nabla \vec{v}^T \right) - \frac{2}{3} \nabla \cdot \vec{v} I \right], \quad (7)$$

where μ is the molecular viscosity, I is the unit tensor, and the second term on the right hand side is the effect of volume dilation.

The developed model was solved using a Fluent Solver. The Spalart–Allmaras turbulence model was considered the turbulence model, and the boundary conditions with inlet velocities of 1 m/s, 5 m/s, and 10 m/s and ambient pressure of 1 atm were employed with air as the continuous phase, and the droplets containing the simulated virus particles acted as the discrete phase. Figure 2 shows the vector plot with the continuous phase (air), the discrete phase (viral droplets), and the ambient air. The red colour denotes the maximum distance traveled by the viral droplets. Furthermore, Figure 3 shows the velocity contour of air ejected from the inlet (mouth) with an initial velocity of 5 m/s.

3. Results

The contour of the distance traveled by the droplets for the considered initial velocities is shown in Figures 4(a)–4(c). Figures 5(a)–5(c) show the contour of the droplets' velocity. Finally, the distance traveled by the simulated viral droplets in response to various initial velocities is shown as a function of time in Figures 6(a)–6(c). Results demonstrate that the maximum distance traveled by the particles for the initial velocities of 1 m/s, 5 m/s, and 10 m/s is 0.64 m, 1.07 m, and 1.24 m, respectively.

Figures 7(a)–7(c) show the decrement in the velocity of the simulated viral droplets (with an initial velocity of 1 m/s, 5 m/s, and 10 m/s) as a function of time in seconds. It is observed that the velocity of the droplets decreases exponentially as a function of time within a maximum of 1-second interval. Furthermore, Figures 8(a)–8(c) show the change in velocity of the viral droplets as a function of the distance traveled by the particles with initial velocities of 1 m/s, 5 m/s, and 10 m/s, respectively. It is seen that the droplets traveling with the initial velocities of 1 m/s, 5 m/s, and 10 m/s lose their significant velocities at a distance of 0.64 m, 1.07 m, and 1.24 m, respectively.

4. Discussion

Human activities such as cough, sneezing, and nasal and oral breathing expel droplets which act as vectors or mediums to transmit the infection from person to person. Expelling the droplets through the tubular structure, including the mouth's contour, follows the jet turbulence. Direct numerical simulation is the best option to model the turbulence as it resolves eddies of all length scales. When a person voluntarily coughs, droplets of different sizes are expelled through the mouth mostly and to some extent through the nose. When a person speaks, salivary droplets containing the infective particles from the throat are expelled through the mouth. While the reflex of cough or sneezing expels the droplets in seconds, speaking expels droplets for a more extended period. Such droplets are responsible for person-to-person transmission through aerosol routes. Though the droplets in the range of 5 to 10-micron size are considered responsible for airborne transmission [19, 20], there is no

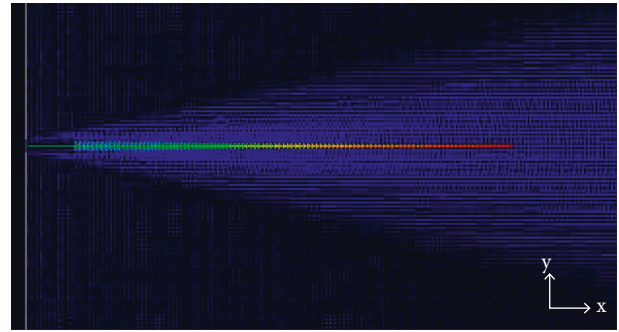


FIGURE 2: Vector plot of continuous phase and discrete phase. The discrete phase model is a turbulence model which is used for tracking particles in the air. The flow of air is the continuous phase and simulated droplets are denoted as the discrete phase.

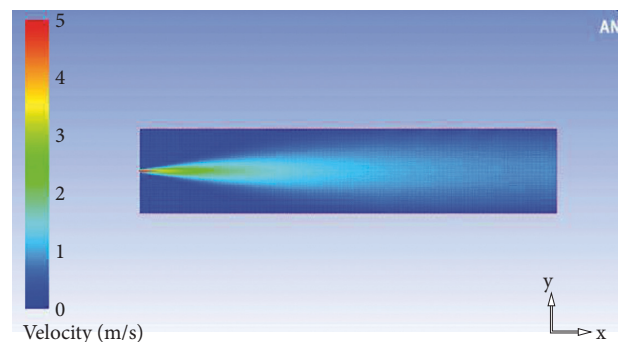


FIGURE 3: The velocity contour of air issued from the inlet (mouth) at 5 m/s. The initial velocity and the changes in velocity represented by different colours represent the velocity contour of the simulation.

consensus on this critical parameter of droplet infection. While some authors consider a size larger than $20\ \mu\text{m}$ as droplets, others consider that only droplets larger than $60\ \mu\text{m}$ can sustain and cause droplet infection [7, 21, 22].

Blocken et al. [23] analyzed the aerosol SARS-CoV-2 transmission for an individual walking or running after another individual using the Ansys Fluent software. The authors concluded that the rear individual is highly exposed to the front individual's droplets. Dbouk and Drikakis [24] used OpenFOAM software to analyze aerosol transmission by human cough during high/slow wind speed. The authors demonstrated that for a wind speed of 4–15 km/h, the droplets can move up to 6 m from the affected individual.

It has been estimated by particle image velocimetry that the average velocity of air expelled by coughing and speaking was 11.7 m/s and 3.9 m/s, respectively. The authors also estimated that each act of cough and speaking expelled 947 to 2085 and 112 to 6720 droplets, respectively [9]. Real-time shadowgraph imaging for pepper stimulus showed that the maximum sneeze velocity was 4.5 m/s, and droplets traveled up to 0.6 m [2]. However, the act of cough during acute inflammation of the upper respiratory tract is expected to expel more force than in the experimental situation. Cough is a forcible involuntary act in response to the inflammation of the upper and lower respiratory tract. It can also be considered a good sign from an individual perspective as the

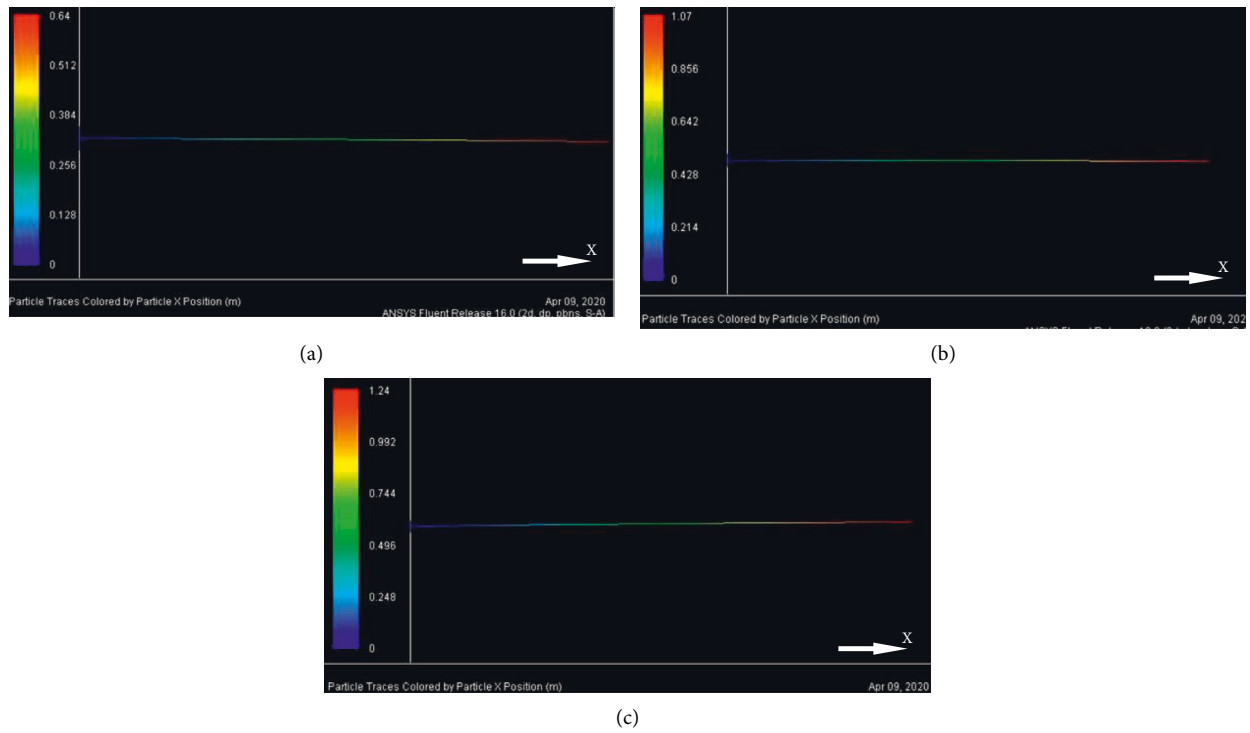


FIGURE 4: Colour plot showing the contour of the distance (in meters) traveled by the simulated viral droplet with initial velocity of (a) 1 m/s, (b) 5 m/s, and (c) 10 m/s.

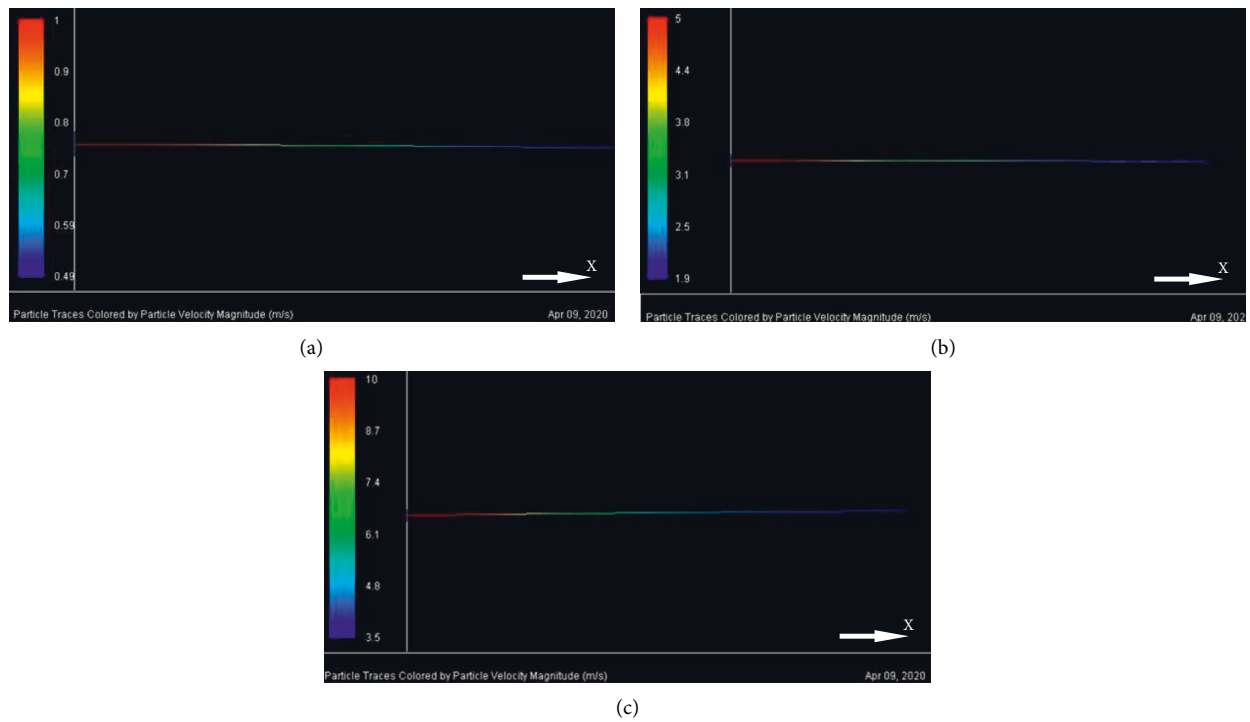


FIGURE 5: Colour plot showing the velocity contour (m/s) of the simulated viral droplet with initial velocity of (a) 1 m/s, (b) 5 m/s, and (c) 10 m/s.

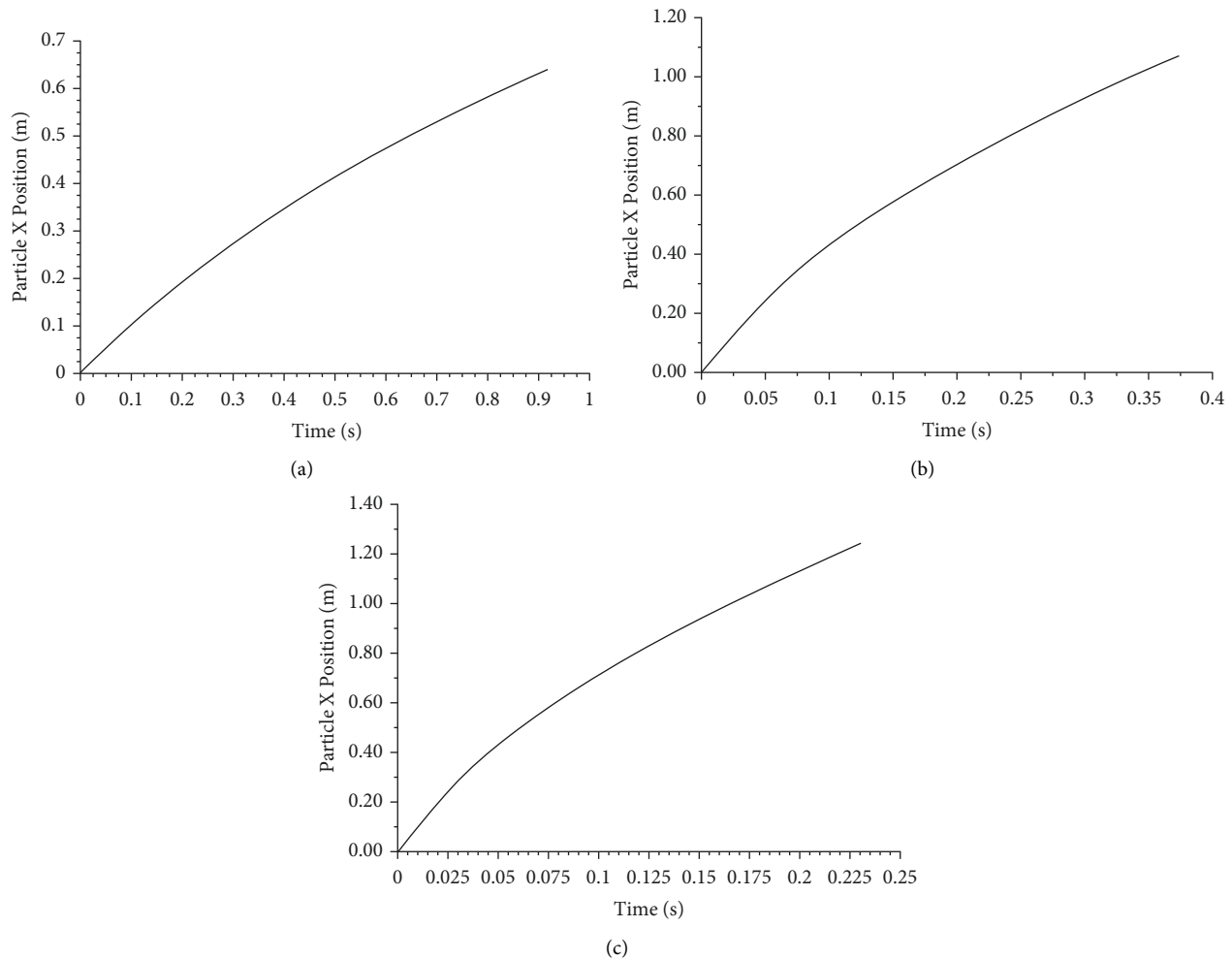


FIGURE 6: The distance traveled by the viral droplets with initial velocities of (a) 1 m/s, (b) 5 m/s, and (c) 10 m/s, shown as a function of time. The maximum distance traveled by the simulated droplet depends on the initial velocity. When the initial velocity increases, the time taken to reach the maximum distance reduces. For an initial velocity of 1 m/s, the droplet takes about 1 s to reach the maximum distance, whereas the droplets with initial velocity of 5 m/s and 10 m/s take 0.35 s and 0.23 s, respectively, to reach the maximum distance.

system attempts to expel the virus particles. However, from a public health perspective, it endangers transmission, and the transmission potential depends on the size of the particles, the distance traveled, and the surface on which the droplets stick. It has been shown that the expulsive phase of cough with speed up to 100 km/h [25] generates droplets of various sizes containing components from all the tubular structures of the respiratory tract.

Several studies have shown similar results for the velocity of the droplets expelled from the acts of coughing and speaking. However, the results on the droplet sizes varied widely. In our experiment, we have simulated the droplet size of 10 microns as it has already been shown that droplets between 8 to 16 microns constitute a significant part of the cough and sneeze as these droplets are expected to play a significant role in airborne transmission during a brief period of contact, in particular in working environments such as call centers, laboratories, hospitals, libraries, and shopping counters. In a closed environment, in particular, under an air-conditioned roof, speaking by asymptomatic persons is likely to expel a constant stream of droplets for a

short distance leading to unrecognized community SARS virus transmission. Recent COVID-19 transmission experience in Chennai, India, had shown that one cashier in a shopping mall was infected when she came in brief contact with the two infected travelers from Kerala. These infected persons were asymptomatic, and therefore the droplets during the act of conversation must have resulted in successful transmission. Medical professionals advocate two-hand length distances in clinical practice to prevent closed-door transmission [7]. This principle was applied in hospitals to place the adjacent beds and design the breadth of the wards (5-6 meters) in the general wards where patients with different diseases are treated. In the current COVID-19 pandemic, these simple principles practiced in infection containment are very relevant and essential in quarantine camps. In our experiment, the numerical model predicted that with the initial velocities of 5 m/s and 10 m/s, the droplets can travel up to 1.07 m and 1.24 m, respectively. When the initial velocity was increased to 30 m/s, the simulated viral droplets can travel up to 2.51 meters as analyzed using the regression model, as shown in Figure 9.

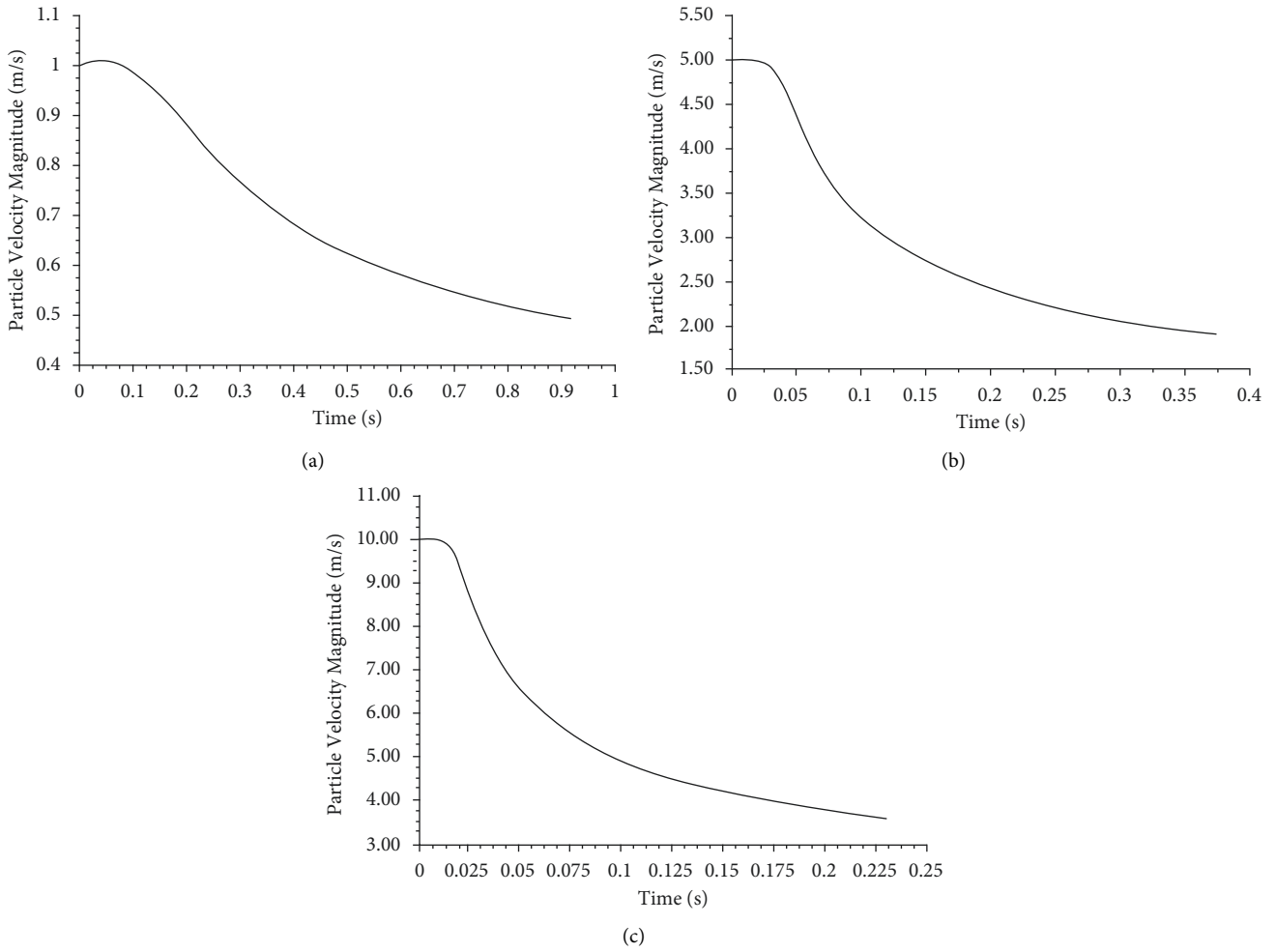


FIGURE 7: The velocity of the viral droplets with initial velocities of (a) 1 m/s, (b) 5 m/s, and (c) 10 m/s, shown as a function of time. The droplets have higher velocity when they are ejected from inlet (mouth), and with the progression of time, the momentum begins to decrease rapidly.

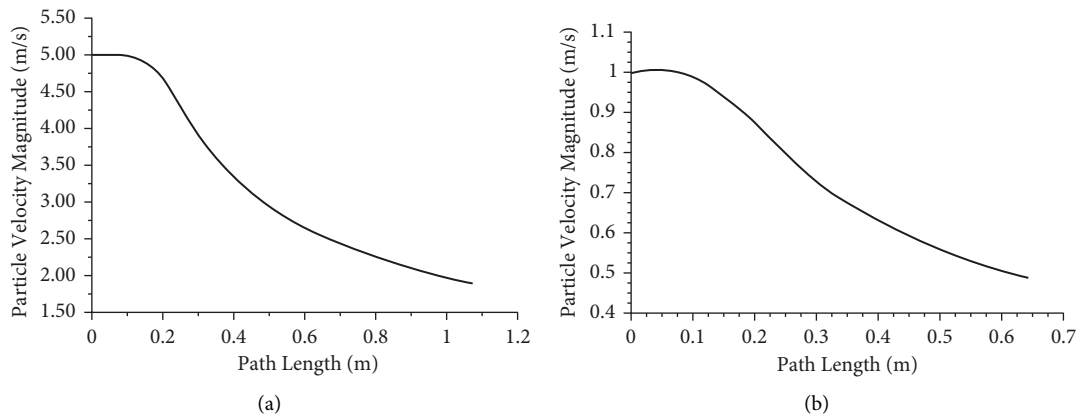


FIGURE 8: Continued.

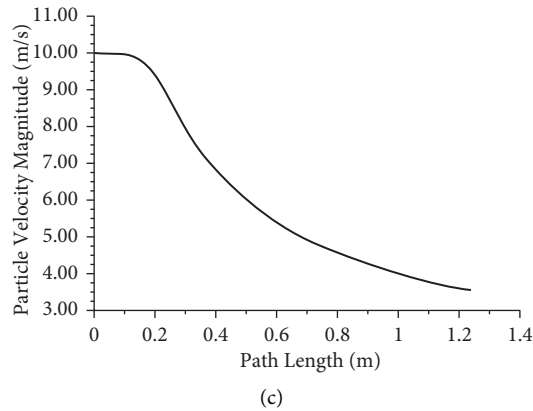


FIGURE 8: The velocity of the viral particles (with initial velocity of (a) 1 m/s, (b) 5 m/s, and (c) 10 m/s) shown as a function of the distance traveled by the particles. The droplet with initial velocity of 1 m/s travels up to 0.64 m while the droplet with initial velocity of 5 m/s and 10 m/s travels up to 1.07 m and 1.24 m, respectively.

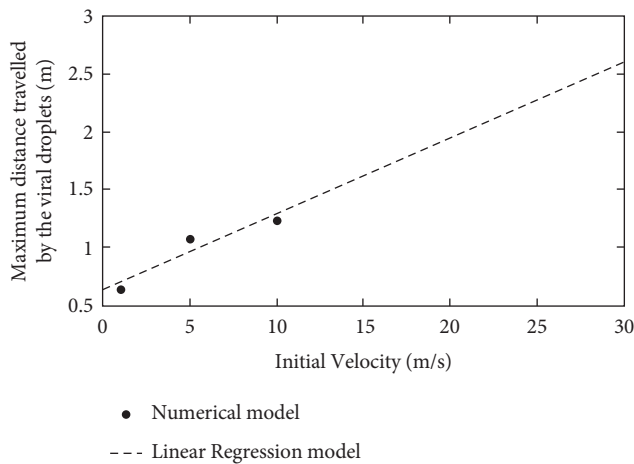


FIGURE 9: The maximum distance traveled by the simulated viral droplets as a function of initial velocities in the range of 1 to 30 m/s. It is observed that the viral droplets travel a maximum distance of 2.595 meters for an initial velocity of 30 m/s.

5. Conclusions

Computational modeling plays a vital role in biology and medical sciences. It is widely applied in designing the cardiac valves, refining laser surgical techniques, drug discovery, and drug administration. This work developed a realistic computational model for transmitting SARS-like viruses, including the novel CoV2, through the ambient atmosphere with ambient atmospheric forces. The model was numerically simulated using various inputs of the initial velocities comparable to the acts of coughing, sneezing, and speaking. Results demonstrate that the developed model performs efficiently and can assess the distances traveled by the simulated particles of 10-micron size through the atmosphere. A particle image velocimetry (PIV) study by Zhu et al. showed that the initial cough velocity was 22 m/s for average persons [26]. By 3D numerical simulation, Dbouk and Drikakis [24] demonstrated that the environmental condition, in particular the wind speed, influences the

dispersion of droplets up to six meters [27]. Depending on the RH, temperature, and wind speed, the infective droplets can infect persons up to 10 feet in the distance [28]. In addition, acute inflammation's blockage of the respiratory tract considerably impacts droplet dispersion. Nasal blockage can lead to a 300% rise in droplet contents at six feet and a 60% increase in droplet dispersion distance [29]. In the current study, we checked for the transmission potential of viral droplets in indoor conditions as experienced in India. We elsewhere indicated that COVID-19 transmission was high during social gatherings in a closed environment. We simulated and tested the distance traveled by droplets of 10-micron size under ambient conditions with an initial velocity of 5 m/s, 10 m/s, and 30 m/s in the ambient conditions. The total distance traveled by the simulated viral droplets for an initial velocity of 30 m/s was 2.51 meters.

These results are relevant in the current COVID-19 pandemic and the continued threat with several variants such as Delta, Omicron, and XE variants in India. They have practical applications in the transmission at quarantine camps, institutions, hospitals, and public places. While the World Health Organization recommends at least 1 meter as social distancing for preventing transmission from cough and sneeze [30], the CDC recommends 6 feet or 2 meters [31]. However, modeling studies have demonstrated 23% median reduction in the cumulative attack rate of influenza infection in the general population [32, 33], but there is a paucity of information from community studies. It is challenging to conduct community studies on social distancing to identify optimal social distance. However, institutional studies can determine the impact of novel CoV2 transmission in different social distancing strategies. Until we obtain the results of such institutional studies, the computational studies provide valuable information on social distancing. In addition, maintaining a social distance of 2.5 meters is not feasible in public places and closed transport systems. Though the mask's efficacy in filtering the virus particles is debatable, it has been shown that even a homemade mask coupled with hand hygiene effectively reduced the novel CoV2 aerosol transmission [34], and

several countries advocate these practices. Therefore, wearing masks in community containment zones must be encouraged to prevent droplet and aerosol novel CoV2 transmission. It is established now that SARS-CoV-2 goes through several mutations, and vaccines prevent the severity of the disease, not the reinfection. Therefore, prevention measures such as social distancing and facial masks need to be encouraged to prevent the SARS-CoV-2 epidemic waves in local settings and international spread.

Data Availability

The data utilized for model development of this study are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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