Developing an infectiousness model for droplet transmission

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Abstract. Modelling of droplet based transmission in clinical spaces guided by a combination of the principles of medicine and physics can produce safer environments. Understanding airborne respiratory disease transmission is essential in light of the recent worldwide SARS-CoV-2 pandemic. This can help define better public health strategies to adopt and to design public spaces in such a way that humanity is less vulnerable to airborne transmission. Airborne infectious saliva droplets are the principal factor of transmission and the infectiousness is associated with the magnitude of the viral load. There is a need to consider the effects of local environmental factors on the evolution of droplet infectiousness. This work presents a computational fluid dynamics (CFD) model that incorporates heat and mass transfer to account for droplet evaporation. An Eulerian-Lagrangian approach was used to simulate air and particle flow. These flows were calculated using a two-way coupling method. Interactions between droplets are captured with coalescence and breakup models. The model assumes infectiousness is proportional to droplet volume which here has a constant pathogen concentration in the saliva. Results from this work show that higher temperature lowers infectiousness of the droplets containing the virus by increasing their evaporation, whereas humidity considerably reduces their evaporation rate and thus sustains their infectiousness. Thus ideally indoor spaces should be warmer, drier and ventilated. The results are benchmarked to measurement and other computational based methods and studies. The aim is to use the model to optimise the design of clinical and public spaces with optimal ventilation to minimise risks of infection.

1. Introduction

Airborne respiratory diseases are affecting humanity and can even turn into a global pandemic. Policies which ameliorate the infectiousness of the droplets need to be set in public spaces. For that, a better understanding of the physical phenomena occuring during the air-carriage of respiratory droplets responsible of disease transmission is crucial. During the recent SARS-COV-2 pandemic, researchers investigated this matter and different approaches can be found in literature : experimental [1, 2], theorical [3, 4] and computational studies [5, 6].

In this study, we consider the case of SARS-CoV-2 and Tuberculosis and similar, where pathogens are contained in expelled saliva droplets which are driven by the local air and are influenced by environmental factors. The infectiousness of a SARS-COV-2 droplet is proportional to its viral load count, with higher viral loads increasing ones susceptibility to infection. For a single droplet, the higher the viral load, the higher its infectiousness. Saliva droplet size decreases with time due to evaporation. Hence, the number of pathogens would decrease as the droplet evaporates, as described in reference [7], where it is assumed that pathogens leave the droplet at the same rate as the fluid, and that dry pathogens are soon rendered harmless. Infectiousness is then decreasing with droplet volume. In this study, the main objective is to develop an infectiousness model that accounts decreasing droplet infectiousness due to air flow and environmental factors (temperature and humidity).

2. Modeling approach

The model computes air and particles in such a way that air and droplets are coupled. Air motion is impacting on particles and impacts of particles are also incorporated in the air equations.

2.1. Euler-Lagrange approach

Air flow and droplet motion are coupled using the Euler-Lagrange approach. Air is considered as a continuum and is computed with the Navier-Stokes equations :

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = S_m \tag{1}$$

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial u_l}{\partial x_l}\right)\right] + \frac{\partial}{\partial x_j}\left(-\rho\overline{u_i' u_j'}\right) + S \tag{2}$$

where ρ, u_i, S_m, p, μ, u_i' and S are density, mean velocity, mass source, pressure, dynamic viscosity, velocity fluctuations and momentum source of air respectively ; δ_{ij} is the Kronecker delta.

Turbulence is treated with the Shear-Stress Transport (SST) $k-\omega$ model. The Reynolds stresses $-\rho\overline{u_i' u_j'}$ are modeled with the Boussinesq hypothesis and the turbulent kinetic energy k and the specific dissipation rate ω transport equations are added as described in reference [8].

Droplets are considered as a discrete phase and their trajectories are computed by integrating the force balance on the particles :

$$\frac{d\vec{u}_p}{dt} = \frac{18\mu}{\rho_p d_p^2}\frac{C_D}{24}\frac{\rho d_p}{\mu}(\vec{u} - \vec{u}_p) + \frac{\rho_p - \rho}{\rho_p}\vec{g} \tag{3}$$

where $\frac{18\mu}{\rho_p d_p^2}\frac{C_D Re}{24}(\vec{u} - \vec{u}_p)$ is the drag force per unit mass, C_D is the drag coefficient, $\vec{u}_p$ is the particle velocity, ρ_p is the particle density and d_p is the particle diameter.

To account for the effect of turbulence on particle motion, a turbulent dispersion model is used. The fluid velovity u is then equal to $\bar{u} + u'$. More complex particle-particle interactions ware also taken into consideration by adding broplet breakup and coalescence models.

The two-way coupling approach is used to enable momentum, heat and mass exchange between air and droplets. While the droplet trajectory is calculated, gain or loss of heat, mass and momentum are tracked. Those quantities are then incorporated in the air equations as sources. Air and droplets are then impacting each other. As described in reference [8] heat and mass transfer law between air and particles depends on the particle temperature T_p. If the droplet temperature is lower than the vaporization temperature or if the volatile fraction of the droplet is fully consumed, the following equation is solved :

$$m_p C_p \frac{dT_p}{dt} = hA_p(T_\infty - T_p) + \varepsilon_p A_p \sigma(\theta_R^4 - T_p^4) \tag{4}$$

where m_p, C_p, A_p and ε_p are the particle mass, heat capacity, surface area and emissivity, T_∞ is the temperature of air, h is the convective heat transfer coefficient, σ is the Stefan-Boltzmann constant and θ_R is the radiation temperature.

When the particle temperature reaches the vaporization temperature, the droplet is vaporizing and transfer mass to the continuous phase. The following equations are computed until the volatile fraction of the droplet is fully drained :

$$N_i = k_c(C_{i,s} - Ci,\infty) \tag{5}$$

$$m_p(t+\Delta t) = m_p(t) - N_i A_p M_{w,i} \Delta t \tag{6}$$

where N_i is the molar flux of vapor, k_c is the mass transfer coefficient, $C_{i,s}$ is the vapor concentration of the droplet surface, $C_{i,\infty}$ is the vapor concentration in the air and $M_{w,i}$ is the molecular weight of the vapor.

2.2. Injection properties

The way droplets are expelled is described by some parameters : the injection velocity and temperature, the size distribution of the droplets, and the droplet flow rate. Those properties depend on the respiratory event taken into consideration, whether it is a breathing, coughing or sneezing. In this study, we are considering a cough as described in reference [9]. The injection surface is rectangular shaped, its sides are 4 cm and 0.48 cm. Droplets are injected at a temperature of 34°C. The cough period is of 0.12 s, and the flow rate is calculated in order to obtain a total injected mass of 7.7 mg. Droplets are injected at a velocity of 11 m/s, which is the average velocity of a cough as indicated in reference [10].

The particle diameter follows a Rosin-Rammler distribution given by the following equation :

$$f(d) = e^{\left(-\frac{d}{\bar{d}}\right)^n} \tag{7}$$

where d is the droplet diameter, $f(d)$ is the cumulative mass fraction corresponding to droplet of diameter d, $\bar{d}$ is the mean diameter and is equal to 80 μm, n is called the spread parameter and is equal to 8. The minimum and maximum diameter are respectively 10 μm and 110 μm.

3. Results and discussion

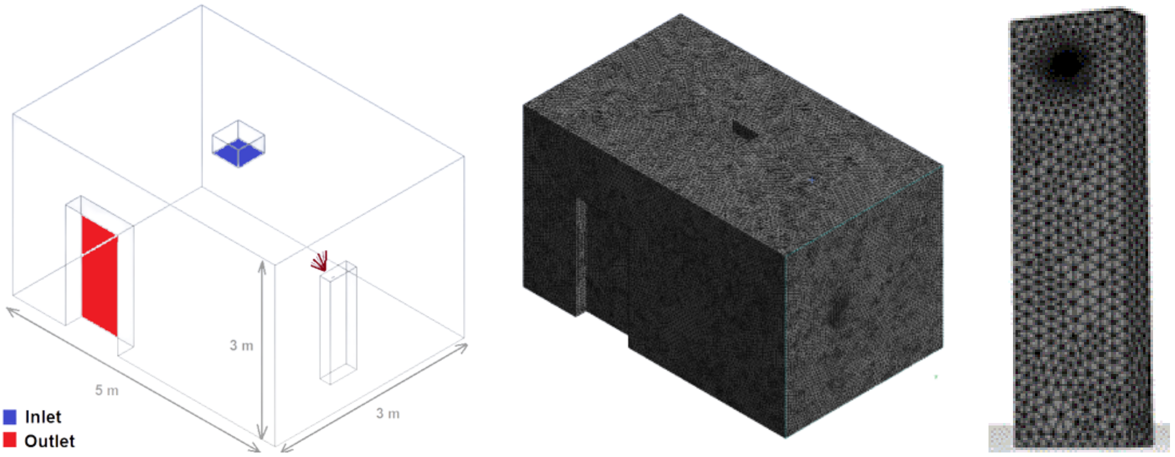
For these preliminary studies, for the purpose of model development and benchmarking, the simulation domain is a simple room with an air vent as an inlet and a door as an outlet (Figure 1a). The cough is released from a rectangular shaped face located at 1.7 m height. The domain was meshed using tetrahedral shaped mesh elements, refined at the injection face (Figure 1b and 1c).

The simulation was run inside this simple room. To highlight the effect of air flow on droplet dispersion, two different cases were investigated. The first one is when there is no air flow inside the room, the other one is when air is flowing. In the last case, the velocity inlet at the air vent was set to 1 m/s. However, the air is experiencing some backflow at the outlet, resulting in the air velocity going up to 5 m/s (Figure 2 (a)). Velocity streamlines from the surface where droplets are injected are plotted in Figure 2 (b), to get an idea of how droplets would be transported.

When particles are expelled in a room with no air flow, particles of diameter $d \leq 3\mu m$ are buoyancy driven and remain airborne (Figure 3 (a)) whereas larger ones ($d \geq 5\mu m$) are more affected by gravity and rapidly fall to the ground. When air velocity is substantial, particles are better dispersed throughout the room (Figure 3 (b)).

The effect of evaporation is also important. The CFD modelling is able to follow this and show evaporation rate is accentuated by temperature (Figure 4 (a)), it is lowered by humidity (Figure 4 (b)) and it is accentuated by relative air flow.

In Figure 5, the pathlines of the droplets are tracked. For simplicity the air flow is zero. The droplets are color coded to their diameter, and it can be seen this diameter decreases due to evaporation. In the left part many droplet pathlines are shown and in the right part only a single one for clarity. This decrease in droplet size by evaporation occurs with a loss of virus. This represents the attenuation of infectiousness

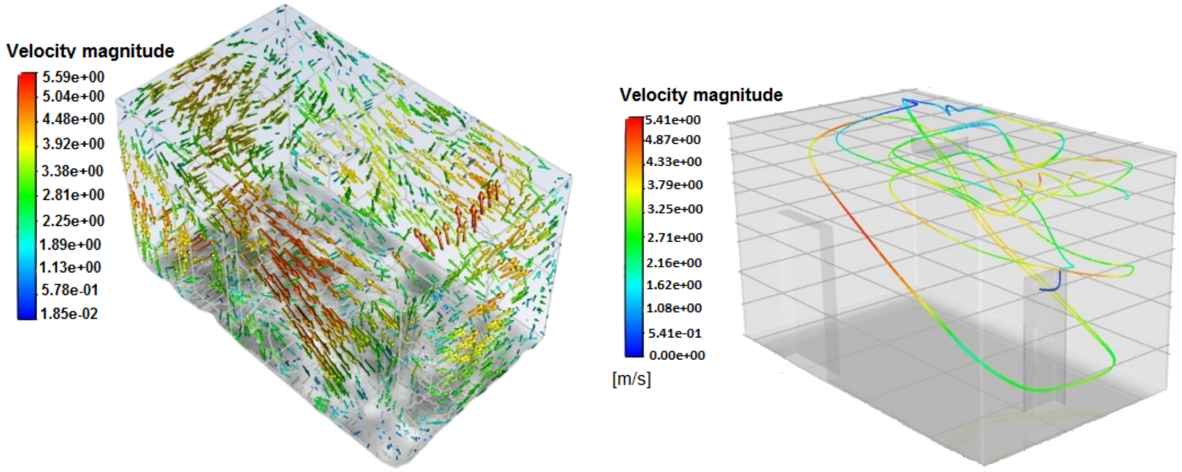


(a) Simulation domain.

(b) Meshed domain.

(c) Finer mesh at injection surface.

Figure 1: The domain and its treatment



(a)

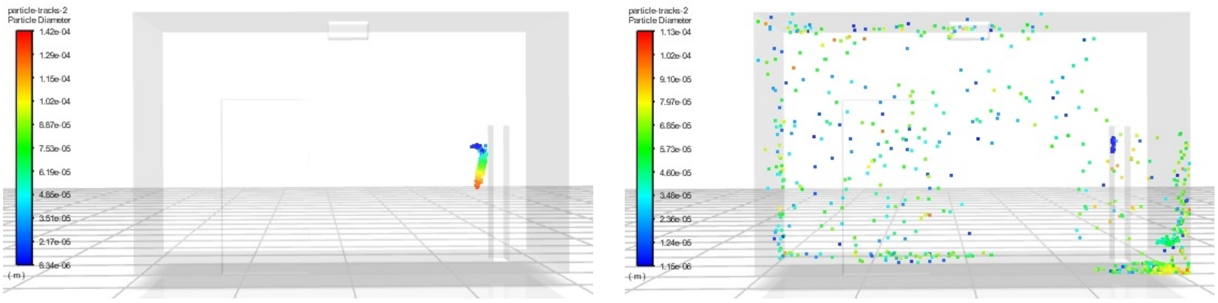
(b)

Figure 2: (a) Air velocity field, (b) air velocity streamlines.

due to decomposition of dehydrated viruses [7]. This then represents the preliminary goal of the study, to incorporate a model for decreasing droplet infectiousness due to evaporation, and to track this on a per droplet basis.

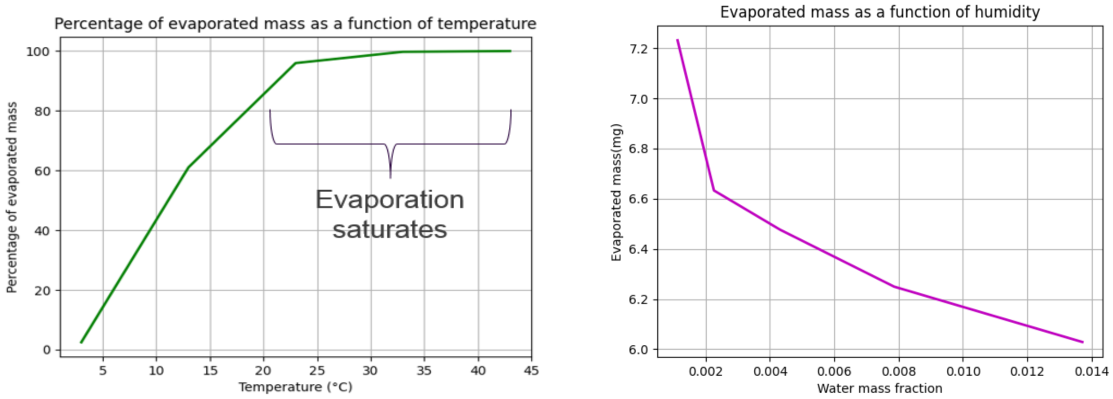
Thus closed spaces, which are likely to keep moisture, would experience lower evaporation, and small airborne particles would last longer. But in ventilated spaces, evaporation would be higher, in Figures 3 (a) and (b) residence time would be lower and droplet infectiousness would decrease [11].

The model is benchmarked to the CFD model in reference [9]. In this paper, particles are injected in an open environment, with wind coming from behind the coughing person. The mouth is located at 1.63 m. Figure 6 shows a result obtained with our model in the case of wind speed being equal to 4 km/h. Distance travelled by droplets for a given time are consistent with results shown in reference [9]. The difference resides in the fact that in our result, particles are more affected by gravity, due to coalescence.



(a) (b)

Figure 3: Particle dispersion (a) in a room without air flow, (b) with air flow.



(a) (b)

Figure 4: Evaporation rate as a function of (a) temperature, (b) humidity.

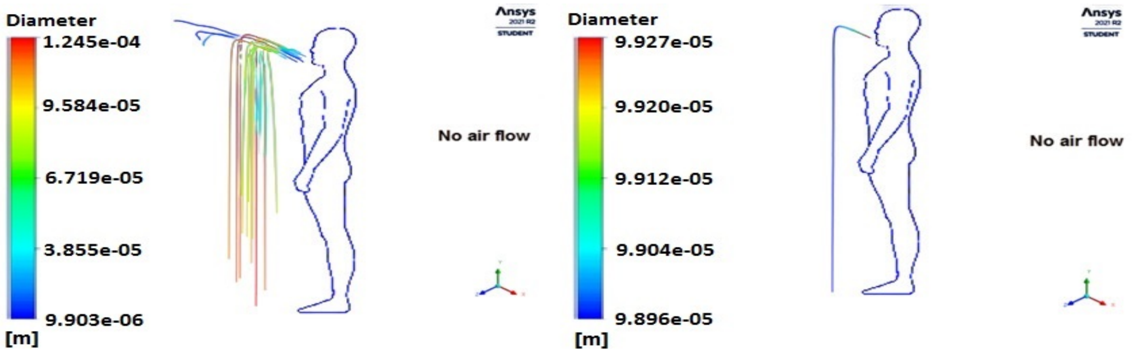


Figure 5: Particle pathlines. In the figure in the right, the decrease in droplet size is shown and therefore infectiousness decreases due to the effect of evaporation.

4. Conclusion

The main goal of this study is to introduce a model for the infectiousness of respiratory diseases transmitted by expelled droplets, into a larger CFD model of the fluid space. The Computational Fluid dynamic model simulates the transport and evolution of droplets expelled from a cough. Particle trajectory is computed in a simplified environment, effect of temperature and humidity of the

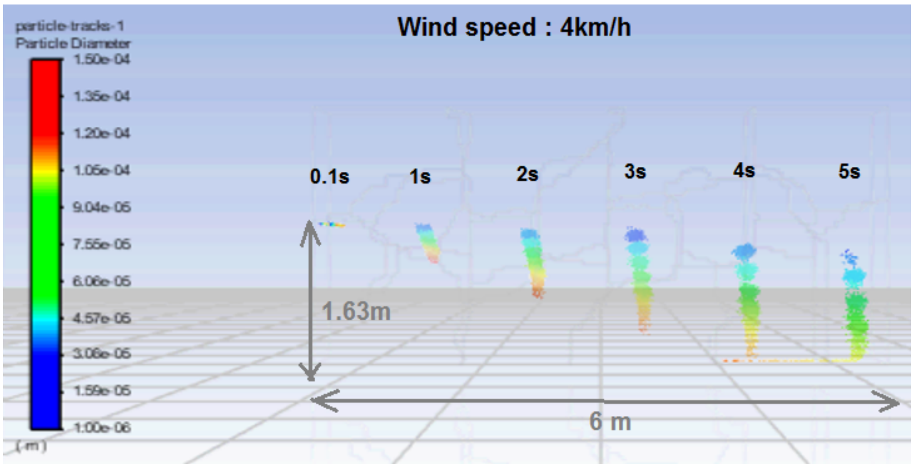


Figure 6: Particle motion in an open space. With wind speed of 4 km/h droplets of diameter $d \leq 4\mu m$ remain airborne and the effect of gravity is causing the larger droplets ($d \geq 100\mu m$) to fall to the ground faster.

environment is taken into account by considering droplet evaporation. The influence of air flow on droplet dispersion is also taken into consideration. It is seen that this scheme is able to track the time evolution of infectiousness of individual droplets.

These findings are critical for public health facilities treating patients with airborne transmissible diseases such as SARS-CoV-2, tuberculosis or influenza amongst others. Such facilities need to be designed to incorporate ways of minimizing the risk of disease transmission by improving ventilation and controlling temperature and humidity. Further studies will deploy this model in selected public and clinical spaces.

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