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EVLING DROPLET DYNAMICS DURING VIOLENT EXPIRATORY EVENTS AT VARIOUS AMBIENT ENVIRONMENTS

F. Gerbino,1 G. Tretola,1 R. Morgan,1 P. Atkins,1 S.J. Waddell,2 S. Pitt,3 & K. Vogiaztaki1,*

1Advanced Engineering Centre, University of Brighton, Brighton, BN2 4AT, United Kingdom
2Department of Global Health and Infection, Brighton and Sussex Medical School, University of Sussex, Brighton, BN1 9PX, United Kingdom
3School of Pharmacy and Biomolecular Sciences, University of Brighton, BN2 4AT, Brighton, BN1 9PX, United Kingdom

*Address all correspondence to: K. Vogiaztaki, Advanced Engineering Centre, University of Brighton, Brighton, BN2 4AT, United Kingdom, E-mail: k.vogiatzaki@brighton.ac.uk

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In this paper we use simulation techniques to provide new insight into the effect ambient temperature and humidity have on the evolving size and temporal dynamics of the droplets exhaled during coughing and sneezing. Four different temperatures were investigated corresponding to various weather conditions ranging from moderate (T=16°C and 25°C) to more extreme conditions (T=4°C and 45°C with a relative humidity of 30% and 60%). Numerical observations show that regardless of the ambient temperature, the travelled distance of the droplets in sneezing is longer (2.5m) than in coughing (2m). Current WHO guidelines indicate 1.8 m social distancing which might not be thus adequate. We demonstrate-for the first time- that evaporation depends on the gradient of the exhaled air temperature and the surrounding air rather than the ambient temperature itself. Larger droplets are more affected by the ambient conditions since due to gravity leave quicker the exhaled air cloud. Smaller ones are trapped longer to the exhaled air and evaporate quickly due to body temperature initial conditions. An additional important finding is that in both events, the droplet clouds evolve towards lower Stokes numbers supporting the hypothesis for increased aerosol transmission risk as time proceeds. Our work contributes to the better mapping of the droplet sizes and transmission route offering information hard to acquire experimentally for their dynamics in different times. These results help to guide public health policies to reduce the transmission of respiratory diseases, confirming the importance of social distancing to prevent them.

KEY WORDS: sneeze, cough, droplet dispersion, spray, OpenFOAM, Eulerian-Lagrangian

1. INTRODUCTION

Respiratory infectious diseases, such as influenza, tuberculosis and severe acute respiratory syndrome (SARS), including the recent SARS-CoV-2 coronavirus, pose a considerable threat for the
life and livelihood of millions of people around the world. Studying the transmission of infectious respiratory diseases is essential to predict and control the transmission of pathogens, such as *Mycobacterium tuberculosis* which is the leading bacterial cause of death worldwide (Nardell, 2015). Transmission mechanisms remain poorly understood. Respiratory infections are transmitted through saliva droplets of different sizes. Based on the World Health Organisation’s (WHO) current terminology (WHO, 2020a), when the droplet particles are $d_p > 5 - 10 \mu m$ in diameter they are referred to as "respiratory droplets" while when they are $< 5 \mu m$ in diameter they are referred to as "droplet nuclei". Smaller droplets have the potential for long-range transmission and they better penetrate the respiratory tract, reaching deeper target tissues within the lungs (Guo et al., 2020). This is why, although they carry less infectious particles, they contribute greatly to the spread of the infectious diseases. The distance which droplets of various sizes can travel is related to how far droplet-borne diseases can transmit.

Based on this distinction between the properties of exhaled droplets, the scientific community considers two main routes for the transmission of respiratory infections. Transmission through respiratory droplets can occur when a person is in close contact (current guidelines by WHO (2020b) indicate within 1.8 metre) with an infected person who has respiratory symptoms (e.g. coughing or sneezing). In such case respiratory droplets that include microbes can immediately reach the mouth, nose or eyes of a susceptible person and result in transmission and new infection. The airborne transmission route is different from droplet transmission as it refers to any pathogen that can be transmitted via droplet nuclei (i.e. aerosols) that remain infectious when suspended in air, usually over greater distances and time.

The characterisation of the transmission mechanisms for different pathogens is an open research question and sometimes an issue of controversy. For example, it was initially suggested by WHO that SARS-CoV-2 was not airborne (WHO, 2020a) however more recently, the possibility for airborne transmission was re-evaluated in various settings especially indoors (Asadi et al., 2020; Morawska and Cao, 2020; Smith et al., 2020). One of the reasons that this ambiguity exists is because it is challenging to define in a consistent manner the various respiratory droplet sizes and how they link to transmission.

A distinction between "small" and "large" droplets is based on the time that droplets remain airborne considering how their trajectory is affected by the dynamics of the surrounding air instead of dependence on their absolute size (Vuorinen et al., 2020). It has been suggested that small droplets stay airborne for significantly long times (e.g. tens of seconds to minutes). These droplets also dry into droplet nuclei very rapidly (tenths of a second). Precise size cutoffs are affected by the ambient conditions. The importance of ambient ventilation and air flow patterns has already been investigated extensively in recent years (Feng et al., 2020; Pendar and Pascoa, 2020; Vuorinen et al., 2020). For example, under still ambient conditions $d_p \leq 200 \mu m$ droplets could be considered to be "small" enough to contribute to the airborne transmission route given that their Stokes number is well below one and their droplet kinematic time scale is less than the sedimentation time (Vuorinen et al., 2020). For more discussion about the size limits for a small droplet, see Xie et al. (2007). The movement of larger droplets, greater than $200 \mu m$, is mainly determined by gravitational settling and to lesser extent by the ambient air flow.

Another important aspect not yet fully understood is the effect of ambient temperatures and humidity on respiratory transmission and this will be the subject of our work. A number of epidemiological studies (Lowen, 2014; Marr et al., 2019) have revealed associations between, for example, influenza and local conditions of humidity and temperature. It was found that transmission was more efficient at lower temperatures ($5^\circ C$) but was reduced at higher temperatures ($30^\circ C$). Dry conditions ($2\%$ and $35 \%$ relative humidity (r.h.)) were also found to be more favourable...
Evolving droplet dynamics at various ambient environments

for spread than either intermediate (50% r.h.) or high (80% r.h.) relative humidity conditions. In another recent study by Zhao et al. (2020), the authors investigated the propagation of respiratory droplets and aerosol particles generated by speech in a wide range of temperatures (0 to 40°C) and r.h. (0 to 92%). The authors concluded that droplets travelled further (up to three times) in low-temperature and high-humidity environments, whereas the number of aerosol particles increased in high-temperature and low-humidity environments. This was also found to be the case for the conditions investigated by Feng et al. (2020) using numerical simulations.

Although these studies offer evidence for the temperature and humidity influence on transmission it is still unclear the exact mechanism causing this correlation. More specifically it is not yet understood if this link exists because the microbes are immobilised at certain environmental conditions or if there is a change in the fluid dynamic behaviour of the respiratory droplets carrying the pathogens. During the transmission process, droplets are never of constant size because they evaporate rapidly. This change in size also changes their dynamic coupling with the surrounding air and potentially their route of the transmission. Thus, droplets with "intermediate sizes" can contribute to either of the previously described mechanisms depending on the changing local weather conditions. The study proposed here will mainly focus on the droplet dynamics, with minor considerations on the effect of the particles on the ambient air. In this work, using numerical simulations, we provide novel insight into the history of droplet trajectories produced by violent exhalation events, such as coughs and sneezes, at various temperatures and relative humidities. We also provide an analysis based on how the transmission mechanism is evolving due to the change of the size and velocity of the particles following a Stokes number analysis.

2. METHOD

The simulations are performed using the Eulerian-Lagrangian framework. This is the preferred framework in other similar works in the field of fluid dynamics of infectious diseases (Busco et al., 2020; Dbouk and Drikakis, 2020; Pendar and Pascoa, 2020; Zhu et al., 2006). The Lagrangian formulation solves the dispersed liquid phase (saliva droplets), represented by individual parcels, while the Eulerian formulation solves for the gas field properties within every cell. The liquid parcels are traced in the Eulerian field and the gas-phase properties at the droplet location result from the interpolation of the cell properties following the Lagrangian Particle Tracking (LPT) technique. In the LPT the spray is considered as a discrete phase comprising of a large number of parcels that are transported using Newton’s second law. The individual liquid particles’ position and velocity can be obtained by:

$$\frac{dx_p}{dt} = u_p \quad \text{and} \quad \frac{du_p}{dt} = \frac{\Sigma F_i}{m_p} \quad (1)$$

where \(x_p\) and \(u_p\) are the particle position and velocity respectively, \(\Sigma F_i\) is the sum of all the relevant forces acting on the particle (e.g. drag, gravitational, buoyancy, pressure forces, etc.) and \(m_p\) is the particle mass.

The particle drag force \(F_D\) is defined as:

$$F_D = C_D \frac{\pi D^2}{8} \rho_f |u_g - u_p| (u_g - u_p) \quad (2)$$

where \(d_p\) is the droplet diameter and \(C_D\) is the droplet drag coefficient for spherical particles defined as in Putnam (1961).
The Taylor Analogy Breakup (TAB) model has been used to simulate the breakup mechanism of the saliva droplets. The TAB model represents an oscillating and distorting droplet as a mass - spring - damper system (O’Rourke and Amsden, 1987). In this analogy, the surface tension force plays the role of the restoring or stabilising force, the resistance of the “spring” is represented by the liquid viscosity and the gas aerodynamic force is the source of the external destabilising force that leads to break up. The TAB breakup model is valid at all Weber numbers.

The evaporation model used here to account for the effect of the temperature variability is developed by Zuo et al. (2000), based on the ideal gas assumption. It accounts for the vaporisation of the droplets due to the species dispersion occurring at the droplets surface.

The expression for the droplet mass loss is:

\[ \dot{m}_p = -\pi D_p Sh \rho_p D_F l n(1 + X_r) \] (3)

Sh is the Sherwood number, a dimensionless number that represents the ratio of convective to diffusive mass transport. It can also be expressed as a function of the Reynolds and the Schmidt numbers: \( Sh = 2 + 0.6 Re^{1/2} Pr^{1/3} \). The term \( D_F \) is the diffusion coefficient of the liquid species and \( X_r \) is a molar ratio. This ratio accounts for the surface molar fraction \( X_s \) (based on Raoult’s law), and the carrier phase concentration, \( X_c \) following the formula below:

\[ X_r = \frac{X_s - X_c}{1.0 - X_s} \] (4)

The terms \( X_s \) is the mole fractions of the evaporated liquid in the film surrounding the droplet surface.

Four different environment temperatures \( T \) have been investigated, 4°C, 16°C, 25°C and 45°C, with a relative humidity of \( r.h. = 30\% \). For \( T = 45^\circ C \) a condition with a relative humidity of 60% has been also considered, closer to saturation point. This humidity is similar to the one used in the well known experiment of van Doremalen et al. (2020) which assessed the sustainability of SARS-CoV-2 in aerosols (< 5mm at 65% of \%r.h.). This was one of the first experiments that showed that SARS-CoV-2 remained viable and infective for at least 3 h in aerosols and opened the debate on SARS-CoV-2 transmission through long-distance aerosols. Relative humidity in our study has been imposed as an initial condition using the Antoine equation (Thomson, 1946).

3. INITIALISING COUGHING AND SNEEZING EVENTS

Violent expiratory events release multi-phase turbulent clouds that are generally composed of buoyant hot moist air and suspended droplets of various sizes. When these droplets evaporate they form droplet nuclei. In this study we will focus on two of these events: coughing and sneezing. Setting the initial conditions for these numerical simulations is of paramount importance for the accuracy of the predictions of the evolving spray dynamics. The two most important inputs for the simulations are the initial droplet size distributions and the velocity modelling of the airflow from the mouth. Other parameters are also needed for the simulations as input, such as the mass of saliva and the mouth area. The modelling is based on experimental data both for coughing and for sneezing and the injection is performed in still air ambient conditions. The air is exhaled at body temperature, \( T_{body} = 36^\circ C \), and it is expelled with the velocity vector being parallel to the ground, with no opening angle. It is important to note that experiments from different authors show discrepancies for the values of these parameters which can also be due to the
variability of participants characteristics. The following sections describe the initial conditions for coughing and sneezing selected in this study.

3.1 Coughing

Several authors have investigated the coughing process, analysing the size distribution and the velocity of the droplets (Bourouiba et al., 2014; Chao et al., 2009; Dbouk and Drikakis, 2020; Duguid, 1946; Gupta et al., 2019; Scharfman et al., 2016; Xie et al., 2009; Yang et al., 2007; Zayas et al., 2012; Zhu et al., 2006). There is no general agreement for the cough duration (which corresponds to the saliva droplets injection), and the airflow velocity. Experiments by different authors indicate that, on average, cough lasts between 0.12 s (Dbouk and Drikakis, 2020) and 0.7 s (Zayas et al., 2012). Some authors have reported a duration of up to 1 s (Gao and Niu, 2006). Here we selected a total duration of 0.3 s, as indicated by Bourouiba et al. (2014) and Vuorinen et al. (2020), considering also the airflow peak at 0.1 s (Bourouiba et al., 2014).

The airflow velocity has been measured in terms of maximum and average speed. Here we used the values reported by Chao et al. (2009) for male subjects: $v_{C,max} = 13.2 \text{ m/s}$ and $v_{C,avg} = 11.7 \text{ m/s}$. Even if other authors report slightly different values for the maximum airflow velocity, there is a general agreement for the average velocity values in the literature (VanSciver et al., 2011; Zhu et al., 2006). Accounting for all these data, a time-varying inlet velocity is applied at the mouth patch for the cough airflow using a parabolic profile of the velocity versus time. Figure 1a shows the modelled velocity for the coughing event.

![Figure 1a](image1.png)

**FIG. 1:** Velocity (a) and initial droplet size PDF (b) for a coughing event. The initial PDF used here (grey histogram) is based on Chao et al. (2009) experimental findings (black dotted line).

For the initial droplet size various distributions have also been reported in experimental studies (Chao et al., 2009; Xie et al., 2009; Yang et al., 2007; Zayas et al., 2012). In numerical studies the Rosin-Rammler distribution was mostly used (Dbouk and Drikakis, 2020; Pendar and Pascoa, 2020). In our study a distribution based on Chao et al. (2009) has been used for a more realistic representation of the expiratory event. In Figure 1b the modelled initial Probability Density Function (PDF) is presented. The mouth patch is modelled as a rectangular surface, whose area is $A_{mouth,c} = 340 \text{ mm}^2$ (Bourouiba et al., 2014; Gupta et al., 2019), considering a length to height ratio of 8.26, as suggested by Dbouk and Drikakis (2020). The height of the
mouth (i.e. the point of injection) is $h_m = 1.689 \text{[cm]}$. Regarding the mass of saliva exhaled during cough, there are relatively big discrepancies reported among different authors, ranging from 2.2 mg (Zayas et al., 2012) to 22 mg (Xie et al., 2009). We selected the average value 6.7 mg, indicated by Zhu et al. (2006) (also in agreement with Dbouk and Drikakis (2020)), based on experiments analysing adult males.

### 3.2 Sneezing

Sneezing is a more violent expulsion compared to coughing. The velocity of the airflow exhaled by the sneeze is higher than that of breath and cough. Also, the total number of droplets generated during the sneeze is larger than that of other respiratory activities (Duguid, 1946). Previous research (Bourouiba, 2016; Scharfman et al., 2016) has shown that sneezing events result in the generation of a sheet of fluid that expands and then breaks apart in long filaments that destabilise, and finally disperses as a spray of droplets. Another interesting aspect of sneezing is that the break up process depends to a large extent on the elasticity of the exhaled liquid. It has been suggested that the more elastic the fluid, or saliva, the longer the fluid travelled before breaking into droplets.

Not many studies have investigated the characterisation of sneezing events in terms of droplet size distribution and velocity. In Busco et al. (2020) it is reported that the exhalation phase of sneeze can be separated into two parts. The first part consists of the ejection of aerosols and saliva droplets, while during the second part the remaining air in the lungs is expelled, for a total duration of approximately 0.5s. The saliva droplets injection lasts for 0.2s, as reported by Bourouiba et al. (2014) and Scharfman (2016). As for the case of cough, the peak of the airflow velocity is expected at 0.1s (Bourouiba et al., 2014). In our study, the maximum and average airflow velocity for the sneeze have been selected according to Bahl et al. (2020), being $v_{S,\text{max}} = 35 \text{m/s}$ and $v_{S,\text{avg}} = 14 \text{m/s}$. Though, as for cough, there are relevant discrepancies between different experimentalists for both the maximum and average airflow velocity. Accounting for the total sneeze duration and the maximum and the average value of the velocity, a time-varying inlet velocity is applied at the mouth patch for the sneeze airflow using a normal distribution to model it (see Fig. 2).

![FIG. 2: Velocity (a) and initial droplet size PDF (b) for a sneezing event. The initial PDF used here (grey histogram) is based on Han et al. (2013) experimental findings (black dotted line).](image-url)
The droplets initial size distribution is based on experimental data from Han et al. (2013) with some modifications. The initial distribution used here is shown in Figure 2b. Notice that the experimental data by Han et al. (2013) show a bi-modal distribution with a plateau in the droplets distribution within the range $3 \times 10^{-4} \div 6 \times 10^{-4}$ m. Also in Han et al. (2013) the authors do not report the presence of particles with diameters $< 10 \mu m$, while in our model they are accounted, according to what has been reported by other authors (Duguid, 1946; Pendar and Pascoa, 2020; Scharfman, 2016).

The mouth patch has been modelled as a rectangular surface, whose sides are 19x9 mm corresponding to an area of $A_{\text{mouth},s} = 171 \text{[mm}^2]\text{], which is approximately what was measured by Busco et al. (2020). The total mass of saliva exhaled during the sneeze was 7.7 mg.}

4. NUMERICAL SET UP

The computational domain shown in Figure 3 consists of non-uniform hexahedral cells, $\approx 4 \times 10^5$, with a total dimensions of $6 \text{ m} \times 1.5 \text{ m} \times 3 \text{ m}$. The mesh was refined at the mouth-patch and then gradually coarsened in the streamwise flow direction ($x$-direction) with five levels of refinement. As regards the boundaries, no-slip condition is set on the surrounding walls, except for the face on the opposite end with respect to the mouth patch, where zero gradient condition is assigned. Notice that the human body is external to the computational domain.

![FIG. 3: Computational domain used: all sides of the domain are set with no-slip condition, except for the mouth patch, which is the inlet of the exhaled air and the particles of saliva, and the opposite wall (at $x = 6\text{m}$), where zero gradient condition is assigned.]

The Lagrangian particles are injected at the mouth patch setting their initial velocity as zero. The particles are eventually "pushed out" by the air flow.
Simulations were conducted in OpenFOAM \cite{jasak2007}, which is a numerical library employing the finite volume method with 2nd order spatial and temporal accuracy. A compressible flow solver is adopted in this study, in which the continuity, momentum and energy equations are solved. The convection terms are discretised with a second order linear discretization schemes, limited towards a bounded first order upwind scheme in regions of rapidly changing gradients, while linear schemes are used for all the other terms. The time derivatives are discretised using a Crank Nicholson scheme. Simulations were run using an adjustable time step, based on the Courant Friedrichs Lewy criterion \cite{courant1967}, setting \( C_{\text{omax}} = 0.3 \).

The sub-grid stress tensors were modelled using the Smagorinsky model \cite{smagorinsky1963}. Calculations are based on the PISO algorithm, implementing a pressure corrector loop.

5. RESULTS

5.1 Saliva spray macroscopic characterisation

Figure 4 shows saliva penetration resulting from sneezing and coughing events in different ambient conditions, as well as the evaporated mass of saliva over time. Defining the penetration as the distance from the mouth which encompasses 95% of the total mass of the liquid droplets, it can be seen that no major effects are observed varying the temperature and the relative humidity up to 1.5 s. As expected, since sneeze is more violent than cough, the particles travel further distances. After 1.5 s we can see a slightly higher penetration for hotter and relatively dry environments consistent with previous studies \cite{zhao2020}. Notice that the saliva penetration for the cough shows a plateau right after a discontinuity point. This occurs because the bigger particles tends to follow a ballistic trajectory, move quickly because of their higher inertia and eventually hit the ground at a distance which corresponds to the plateau. On the other hand, the small particles left behind remain airborne and keep moving until they overtake such a distance, so that the penetration starts to increase again after 1.5 ms.

The evaporated mass is different for coughing and sneezing, since the mass transfer is linked to the droplet size. Smaller droplets heat quicker than larger droplets and evaporate. The evaporated mass for the cough for all cases is higher than the one for the sneeze, due to the larger population of small droplets characterising cough.

At the initial stages of the process and for the duration of the events, indicated by the red line (0.3 s for cough and 0.5 s for sneeze) the ambient conditions play a minor role, while as the time progresses more noticeable differences are present. The only important difference at initial times is that the vaporisation rate at \( T = 6^\circ C, T = 14^\circ C \) and \( T = 27^\circ C \) is steeper than at \( T = 45^\circ C \) and \( r.h. = 30\% \). This can be seen comparing the slope of the evaporated mass in Figure 4 for \( t \leq 0.5 \) s. The lowest evaporated mass for both events for the 2s duration is noticed at \( T = 45^\circ C \) and \( r.h. = 60\% \). For this case humidity is high, closer to saturation, preventing saliva evaporation. Aside from this case, for latter times for the sneeze the evaporated mass increases with increased temperature. For cough the link with the temperature is not so clear. For example at \( t=2 \) s at \( T = 14^\circ C \) the total evaporated mass is much higher than \( T = 45^\circ C \).

To understand the differences in the evaporation between the two events as well as the effect of the ambient temperatures we must consider that initially the droplet clouds are surrounded by the exhaled air of \( 36^\circ C \). This is why at initial stages the evaporation is similar at all temperatures. Then as the event progresses the air coming from the mouth starts to exchange heat with the ambient air. The heat transfer process is better illustrated in Figure 5 where the contour of \( T = T_{\text{body}} = 36^\circ C \) at \( t = 0.25 \) s is plotted. For the cases with lower ambient temperatures, the
region of air remaining at 36°C is more limited than \( T = 45°C \). This indicates that in a colder environment a higher number of droplets are exposed to higher gradient of temperature with respect to the case with \( T_{amb} = 45°C \). This potentially explains why in both events initially the case with \( T = 45°C \) presents lower evaporated mass in comparison to the cases with the same humidity but lower temperatures. As the mixing processes of the exhaled air and the surroundings continues (after 1 s) we can see that in both events and regardless of the temperature (aside of the case of \( T = 45°C \)) the evaporation rate reduced (slope of the evaporated mass) as the temperature gradients are amplified.

These are important finding since although in most studies the environmental temperature is suggested as controlling factor, our study reveals that the evaporation is controlled by how quickly the droplets escape the air cloud coming from the mouth and how quickly the two streams of air (the one from the air and the one from the mouth) mix. In our study considering the surrounding air still we mostly report on the effect of the temperature gradients. However, in more realistic scenarios the ambient air movement will not only affect directly the droplet dynamics but also their evaporation altering further their size.

Other interesting conclusions can be extracted also from Figure 5. In both events smaller droplets follow the trajectory of “body temperature” exhaled air stream while larger droplets are the ones that first become exposed to the ambient temperature environment due to gravity. This reveals that smaller droplets evaporate mostly under the effect of the exhaled air temperature while larger droplet evaporation is controlled by the ambient temperature

**FIG. 4:** Spray penetration at different temperature environment and vaporised mass of saliva; the orthogonal lines show the end of air exhalation (at 0.3s for the cough and 0.5s for the sneeze)

Figure 6 shows the Sauter Mean Diameter (SMD) for sneezing and coughing. It can be seen that overall sneezing produces and maintains larger particles. For both events we can see that as
FIG. 5: Comparison of the temperature contour plot during cough for $T = 45^\circ C$, $T = 14^\circ C$ and $T = 6^\circ C$ (r.h. = 30%) at $t = 0.25s$. The black contour encompasses the gas region where the temperature is $36^\circ C$. The particles’ size represents the relative dimension of the droplets of saliva.

FIG. 6: $D_{32}$ (SMD) over time calculated at different ambient conditions. The events progresses in time the SMD becomes higher. This might appear as counter intuitive given that there is also more evaporated mass generated according to Figure 4. This trend can be explained considering that the smaller droplets which represent the largest population initially, tend to evaporate faster and eventually disappear, leaving (relatively) bigger droplets within the domain and causing the mean diameter to increase with time. This also explains why there is no difference overall in penetration. In fact the penetration reflects that some larger droplets are travelling further downstream. Such a hypothesis is further supported by the observation that for $T = 45^\circ C$ and r.h. = 60%, the higher humidity causes the droplets to evaporate less (i.e. smaller droplets survive longer) and thus the SMD remains smaller than at lower humidity. This is of particular importance because it appears that lower humidity might restrict the airborne mode of transmission although the travelled distance of the larger droplets is the same.

In sneezing, the average diameter remains rather similar for $t \leq 0.5s$ and starts to slightly increase at later times. On the other hand for cough the SMD starts to increase constantly from the very beginning of the injection at a higher rate. This can be explained looking at the droplets initial distribution in Figure 1b and 2b. Notice that the population of small droplets during a cough event is higher than the sneeze (the mode of the diameter is 30$\mu m$ and 81$\mu m$, respectively). These droplets will evaporate faster causing the mean diameter to increase. Further confirmation of this phenomenon is reported in Figure 7. Here, the droplet PDF within the domain during the
cough is shown at $T = 45^\circ C$, with different relative humidity, $r.h. = 30\%$ and $r.h. = 60\%$. The total number of particles as well as the ones with larger diameters decrease as the ambient conditions ($r.h. = 30\%$) promote vaporisation.

**FIG. 7:** Comparison of the droplets diameter PDF within the whole domain at $T = 45^\circ C$ at two different values of relative humidity during cough.

### 5.2 Droplet cloud dynamics

In this section we focus in more detail on the droplet cloud dynamics during the two expiatory events. Although there are differences in terms of ambient conditions, as outlined in the previous section, the trends are similar and thus we only focus on one of simulated conditions ($T = 14^\circ C$ and $r.h. = 30\%$ for both cough and sneeze). The differences in the dynamics between the two events are highlighted.

Figures 8 and 9 demonstrate the dynamics of the saliva droplets at the early time ($t \leq 0.25s$) of ejection from the cough and the sneeze respectively. Droplet sizes between 0.1 to 1000 $\mu m$ are displayed. The colouring has been performed in order to facilitate the distinction of smaller droplets (blue) that are associated with aerosol transmission and larger droplets (yellow and red) that can carry more viral load and cause direct contamination. It should also be pointed out that studies indicate that smaller droplets carry different viral load depending on their origin with the ones resulting from evaporation of larger droplets carrying more load than the ones that directly originate from the mouth (Mao et al., 2020). Thus, it is important to investigate not only their size but their history as well.

Near the mouth a jet profile is observed, which breaks down slowly away from the mouth. The larger droplets start to fall subject to gravity, while the smaller droplets continue following the carrier fluid. Here, we also report the $H_2O$ (saliva) vapour concentration. We use this contour to represent the spreading of the aerosol (particles smaller than 0.1 $\mu m$). In fact, although the simulations account only for the presence of water vapour, in reality saliva contains solid components like salts, cells and microbes, which form droplet nuclei as the water evaporates. Cough tends to produce a vapour cloud more concentrated (green is more intense) and less spread in space, while sneeze aerosols cover longer axial and radial distances. This is consistent with the fact that cough in general produce more small droplets that evaporate quickly while in sneezing due to higher initial inertia and larger droplet sizes this process takes more time allowing the droplets to disperse more before evaporate. We can also see that the vapour concentration spreads radially at the mouth location as the exhaled air impacts the ambient and also interacts...
FIG. 8: Droplet dynamics including the $H_2O$ (saliva) vapour concentration from a human cough. The environment is at ambient temperature of $T = 14^\circ C$ and relative humidity of 30%.

FIG. 9: Droplet dynamics including the $H_2O$ (saliva) vapour concentration from a human sneeze. The environment is at ambient temperature of $T = 14^\circ C$ and relative humidity of 30%.

with the computational domain boundaries. This also causes some droplets (in particular the smaller ones) to travel in a radial direction with respect to the mouth; in fact, the smaller particles ($d_p \leq 10\mu m$) tend to follow the fluid motion due to their low inertia, which in terms of Stokes number indicates the dominance of the advection effects (i.e. the particle “follows” the gas streamline). Due to their small mass, these droplets evaporate quicker creating a pronounced vapour cloud around the mouth. The radial spreading described here is caused by initialisation of the particles, with zero velocity, at the mouth patch. When the airflow due to the expiratory event impacts them, these particles tend to behave as an obstacle and cause the airflow to spread radially. Also, since the mouth patch is surrounded by walls with no-slip conditions, the airflow interacts with them and it is forced to recirculate.

The droplet dynamics in longer times can be observed in Figures 10 and 11 which show the saliva clouds until 2 s. Saliva droplets reach a maximum distance of 1.2 and 2 m for cough and sneeze respectively in the axial direction (from the person’s mouth). The distance and shape of the clouds observed at this interval are of similar order of magnitude from previous studies (Bourouiba, 2016).

*Atomization and Sprays*
Evolving droplet dynamics at various ambient environments

FIG. 10: Evolution of the saliva cloud for a human cough at \( T = 14^\circ\text{C} \) and relative humidity of 30\%.

Droplets with sizes \( d_p \in [100 - 1000]\mu\text{m} \) tend to fall to the ground more rapidly than the rest of the spray, due to their higher weight and thus the droplet cloud appears to be separated. At the upper part reside the smaller droplets while at the lower part larger droplets are found. This is a behaviour that is very hard to be observed experimentally due to resolution limitations, while CFD can report the droplet size composition down to droplet sizes of less than 0.1 \( \mu\text{m} \). The deposition pattern is different between cough and sneeze with cough resulting in particles falling near the injection point although with sneeze the particles deposit in greater length due to their higher initial momentum. The cloud of particles within the \([10 - 100]\mu\text{m}\) range remains in the air a longer time and they reach longer distances (causing the sudden rise which is observed for the saliva penetration in Figure 9). Few droplets with \( d_p \leq 10\mu\text{m} \) are present in the domain, as they vaporise and eventually disappear quickly forming droplet nuclei. The latter class of particles could pose a very high risk for disease transmission as they remain airborne for a long time. Notice in Figure 10 the population of small droplets with \( d_p \leq 10\mu\text{m} \), which are kept at...
FIG. 11: Evolution of the saliva cloud for a human sneeze at $T = 14^\circ$C and relative humidity of 30%.

The simulations performed here refer to an environment of still air, hence no disturbances are accounted for, in terms of wind, airflow, etc. and only gravity affects the droplets. In such simulated environment, the very small droplets will eventually fall on the ground within a relatively short distance. In reality though, these drops may be suspended and advected by the cloud of air emitted by the cougher/sneezer just by breathing or moving. Moreover, the ambient conditions influence the buoyancy of the cloud and therefore the range of contamination caused by its suspended droplets. Changing the buoyancy from summer to winter or indoor conditions can result in variation of the range of deposition of metres for the large droplets, $d_p \geq 100\mu m$, to dozens of metres for the smallest droplets and droplet nuclei with $d_p \leq 10\mu m$ (Bourouiba et al., 2014).

The previous analysis indicated that larger droplets follow a trajectory that is relatively unaffected by the flow in the gas phase, while the smaller droplets are suspended to varying degrees within the turbulent gas cloud. In order to describe numerically how the droplets would be affected by the ambient conditions and in turn their tendency to follow the gas flow motion, it is interesting to analyse the particles in terms of Stokes (St) numbers. The Stokes numbers represent the ratio of the particle inertia to the advection acting on it. $St \gg 1$ indicates the

Atomization and Sprays
dominance of inertial forces while the carrier fluid has limited influence on the particle motion. For \( St < 1 \) the advection effects are more relevant, thus the particles will mostly follow the fluid motion. The mathematical formulation of the \( St \) is the following:

\[
St = \frac{t_0 v_g}{L_0}
\]

where \( t_0 \) is the particle relaxation time, \( v_g \) the gas field velocity magnitude at the particle location and \( L_0 \) a characteristic dimension, which is taken here as the cell size. The relaxation time is defined as:

\[
t_0 = \frac{\rho_l d_p^2}{(18 \mu_g)}
\]

with \( \rho_l \) the saliva density and \( \mu_g \) the air viscosity.

Figures 12 and 13 show the droplet populations in terms of size, velocity and \( St \). The \( St \) numbers are calculated for each particle within the domain at 5 different times: 0.025, 0.1, 0.25, 0.5 and 2 seconds.

**FIG. 12: PDF of the droplets diameter and scatter plot of diameter VS velocity VS St for a cough at four different time steps.**

\[ T = 14^\circ C, \ r.h. = 30\% \]

At any time only few droplets have \( St \gg 1 \), and these are the bigger ones \((d_p \geq 100 \mu m)\), as expected, since \( St \) is proportional to the square of the droplet diameter. The majority of droplets have \( St \sim 1 \). This increases the risk of larger droplet behaving as aerosols that not only stay airborne longer but also curry more viral load. The smaller droplets, with \( d_p \leq 100 \mu m \), have \( St < 1 \) at all times. In both events, the particle clouds evolve towards lower \( St \) values (even for larger remaining droplets) indicating an increased risk of aerosol transmission as time passes.
FIG. 13: PDF of the droplets diameter and scatter plot of diameter VS velocity VS St for a sneeze at four different time steps. $T = 14^\circ C$, r.h. = 30%

progresses. Also at later times the decrease of the Stokes indicates that these droplets are very prone to air disturbances and could be easily moved at far distances by any air movement.

The Stokes analysis brings into the discussion an additional important aspect of the dynamics of the droplet clouds, which is the sedimentation time. The sedimentation time is defined as:

$$t_s = \frac{h}{v_p}$$  \hspace{1cm} (7)

where $h$ is the height of the particle (i.e. its y coordinate) and $v_p$ is the droplet terminal velocity: $v_p = t_0 \cdot g$. Here $g = 9.81 \text{ m/s}^{-2}$ (earth gravitational acceleration) and $t_0$ is the droplet relaxation time defined in Eq.6 to characterise the St number. Such a timescale represents the exponential decay of the particle velocity due to drag.

Figure 14 provides the sedimentation time against the droplet size. It indicates that in still air conditions particles with $d_p \leq 10 \mu m$ remain airborne for more than 30 minutes. As $d_p$ reduces to 1 to 3 $\mu m$, $t_s$ is in the order of tenth of hours, which means that these droplets will eventually evolve into droplet nuclei before reaching the ground. The main difference between cough and sneeze is that for cough there is a wider population of particles which tend to be airborne, due to their small size.

In practice, turbulent flow transports droplets upwards and downwards keeping them suspended in air for sometimes longer, sometimes shorter periods of time than predicted by $t_s$. Note also that the droplet terminal velocity, $v_p$, does not account for the presence of buoyancy force, which could further delay the droplets sedimentation. Since [Bourouba et al. (2014) have

Atomization and Sprays
Evolving droplet dynamics at various ambient environments

5.3 Discussion and comparison with experimental work

To put the simulations presented above into a more realistic context, the simulation results were compared with the experiments from Bourouiba et al. (2014). The simulation and experimental conditions are similar although not identical. The experiments were performed using a high speed camera for $T = 23^\circ C$ and $r.h. = 19.1\%$ (Bourouiba et al., 2014), while the simulations refer to $T = 27^\circ C$ and $r.h. = 30\%$. Another difference is that no initial spray angle has been used in the spray simulations which is expected to cause some discrepancies to the area close to the mouth in terms of spray dispersion. Finally, for cough the duration of the event and the peak are at the same time although the exhalation velocity and droplet size profiles at the mouth area might be different, since these information were not reported in the experimental study.

Figures 15 and 16 compare the saliva cloud evolution obtained from our simulations and the experiments from Bourouiba et al. (2014), for cough and sneeze, respectively. The particle size shown in both these figures for the simulation results represent the relative size of the droplets ejected, while the contour represents the concentration of $H_2O$ (i.e. saliva) vapour. In Figure 15 for the cough event, a shorter cloud penetration is predicted by the simulations. Simulation and experiments agree qualitatively demonstrating larger particles close to the mouth, while smaller particles are ejected further away.

In Figure 16 for the sneezing event, in the first time instances the effect of the spray angle is evident and the droplets in the simulations appear to disperse less. Simulations showed that droplets at $t = 0.34s$ travelled further than what experimentally observed. For $t \geq 0.15s$ particles have a similar trajectory, though the cloud morphology is different. In the simulation the large droplets immediately fall down under the effects of gravity and the smaller ones travel in the sneeze direction. Experimental observations show that large particles are ejected further downstream for $t \approx 0.161s$, while the particle populations differentiate into two different smaller clouds. An important difference to note here, in particular for sneezing, is that we have not considered the head movement, which could enhance the droplets trajectory, as outlined by Busco et al. (2020). To the best of our knowledge, Busco et al. (2020) are the first to report the effects of head motion for sneeze simulation, demonstrating significant differences with the conventional
model with fixed head. Though, [Scharfman et al. (2016)] suggested that the head motion has negligible effects on the timescale of droplets formation and ejection, and considering that in other numerical studies the head motion has not been accounted for (as in [Gao and Niu (2006)] and [Pendar and Pascoa (2020)]), we decided to use the fixed head setup to make the simulations consistent (and comparable) with cough.

**FIG. 15:** Saliva cloud evolution of a cough and relative droplet size spatial distribution obtained from simulations, for $T = 27^\circ C$ and $r.h. = 30\%$ (a). High-speed images of a cough recorded by [Bourouiba et al. (2014)]© at $T = 23^\circ C$ and $r.h. = 19.1\%$ (b).

Simulations were also compared to the experiments in terms of particle trajectory for both cough and sneeze (Figures 17 and 18). In these figures, the experimental control volume is highlighted in green and the trajectories of the largest droplets are included. The colour scheme in the one used for the simulation results in Figures 10 and 11. In general, the behaviour observed in the experiments is well captured by the simulations for both cough and sneeze. The main discrepancy is in sneezing and relates to the spray angle close to the mouth.

For cough, the experiments indicate that the droplets of saliva follow a straight trajectory with a downward angle. On the other hand, the droplets tends to follow a slightly parabolic trajectory in the simulations. In terms of spreading of the trajectories, the experiments and simulations are in agreement. As indicated by [Bourouiba et al. (2014)], the shape of the trajectories suggests a ballistic path for the larger droplets whose dynamics are not greatly affected by the cough cloud. For sneeze, the trajectories obtained by the simulations match well the experimental observations. The droplets tend to follow a parabolic trajectory and this is well captured by the numerical particles. However, the experiments indicate a wider spreading of droplets right
FIG. 16: Saliva cloud evolution of a sneeze and relative droplet size spatial distribution obtained from simulations, for $T = 27^\circ C$ and $r.h. = 30\%$ (a). High-speed images of a sneeze recorded by Bourouiba et al. (2014) at $T = 23^\circ C$ and $r.h. = 19.1\%$ (b).
FIG. 17: Trajectory of the saliva droplets for a human cough at $T = 27^\circ C$ and relative humidity of 30%. The cloud encased in the dotted square is adapted from the experimental results obtained by Bourouiba et al. (2014); such a square region corresponds to their control volume. Note that in Bourouiba et al. (2014) the experimental conditions are $T = 23^\circ C$ and r.h. = 19.1%.

at the mouth exit, as in a “spray cone”. Also, the simulations don’t provide particles moving in the upward direction. The presence of such droplets in the experiments can be related to several factors which are not included in the simulations performed here. In fact, the mouth shape during cough, as well as the position of the lips and tongue could affect the trajectory of the droplets of saliva and are very different for each person.

6. CONCLUSIONS

This paper provides new insight into the effect that ambient conditions, more specifically temperature and humidity, have on the time evolving dynamics of the droplet cloud exhaled during coughing and sneezing. A thorough review of the literature was initially presented to explain the selection process of the initial exhalation conditions for droplet distribution, velocity mouth patch size and exhalation duration. In Eulerian-Lagrangian simulations, as the ones performed
FIG. 18: Trajectory of the saliva droplets for a human sneeze at $T = 27^\circ C$ and relative humidity of 30%. The cloud encased in the dotted square is adapted from the experimental results obtained by Bourouiba et al. (2014); such a square region corresponds to their control volume. Note that in Bourouiba et al. (2014) the experimental conditions are $T = 23^\circ C$ and r.h. = 19.1%.

here, the input parameters affect considerable the accuracy of the results and thus we suggest that it is an aspect of the numerical studies that should be always thoroughly reported when these simulations are used to provide guidelines for social distancing.

Our numerical observations show that regardless of the ambient temperature, the travelled distance of the droplets in sneezing is longer than in coughing. In terms of evaporation rate, for both cough and sneeze, the saliva shows a varying trend with respect to time in respect to ambient conditions. It is unaffected during the events’ duration but shows higher sensitivity to the ambient conditions as the time passes by and the droplets change in size. Overall, the evaporation dynamics were found to depend considerably on the initial droplet dynamics and the temperature gradient between the exhaled air and the ambient conditions.

In terms of cloud dynamics we observed that near the mouth both droplets and the exhaled air follow a jet profile which breaks down slowly away from the mouth. Due to the difference in the Stokes number, particles with different size are subject to different processes. The larger droplets start to fall subject to gravity, while the smaller droplets continue following the carrier fluid. The deposition pattern is different between cough and sneeze with cough resulting in particles falling near the injection point although with sneeze the particles deposit in greater length due to their
higher initial momentum.

In order to describe numerically how much the droplets would be affected by the ambient conditions and in turn their tendency to follow the gas flow motion, we also analysed the particles in terms of Stokes numbers. For both events, the particle clouds evolve towards lower St values indicating the increase of aerosol transmission as time progresses. We also included an analysis for the sedimentation time which revealed that in conditions of still air particles with \( d_p \leq 10 \, \mu m \) tend to remain airborne for more than 30 minutes. As \( d_p \) reduces \( t_s \) gets in the order of tenth of hours, which indicated that these droplets will eventually evolve into droplets nuclei before reaching the ground. The main difference between cough and sneeze is that for the cough there is a wider population of particles which tend to be airborne, due to their small size indicated the higher risk of airborne transmission by coughing event.

Finally a comparison with experimental data from a previous study was performed which indicated a qualitative agreement of the findings, even though there were also noticeable differences underlying the importance of the well defined initial conditions. Several aspects indicated a general agreement between the physical experiments and the simulations. Further experiments are needed to better quantify certain aspects of violent and non-violent expiratory events, in light of the data variability among different experimentalists. It is important to underline that saliva is a non-Newtonian fluid and it has a very variable density and viscosity, depending on the patient, as well as its health conditions. Neglecting this aspect is a limitation of the current model and it needs to be addresses in future studies.

More clarity could inform public health measures designed to reduce the spread of respiratory infections, particularly in enclosed spaces.

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Evolving droplet dynamics at various ambient environments


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