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NUMERICAL SIMULATION OF MULTHIPHASE FLOWS IN THE CONTEXT OF COVID-19/SARS-CoV-2

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Abstract. This research aims at investigate the means of propagation of the COVID-19/SARS-CoV-2 between individuals during social contact. A small scale model is proposed to investigate the behavior of salivary droplets between individuals who may be contaminated by orally transmitted diseases. This will allow a detailed understanding of the rapid spread of COVID-19 viral load and the effectiveness of containment effects of the disease in our society. The results point that saliva particles both travel forward and stay in the air close to a person who coughs.

Keywords: Multi-phase flow, streamfunction-vorticity formulation, BBO equation, particle disperson, finite element method, semi-Lagrangian method

1. INTRODUCTION

In respiratory diseases, the transmission of viral load is almost always carried out through the loading of salivary particles by jets from noses and mouths that reach another individual at a certain distance (Jones (2015)).

Moreover, there's evidence that COVID-19/SARS-CoV-2 spreads not only by direct contact with an infected person, but by airborne transportation of small saliva droplets, which can stay in the air for a long time after they were produced, or be transported for long distances, as suggested by Fineberg (2020). These saliva droplets aren't created only by the 'violent' expiratory events, but also by regular breathing and speech, as evidenced by Asadi S. (2020). This would invalidate current guidelines that state staying 1-2 meters apart from each other and not touching is enough to be safe, without taking into consideration the ambient air people are inserted in. This issue is exacerbated in enclosed and indoor environments, where the air exchange is limited, and for extended periods of exposure time (Morawska (2020))

In this context, this research aims at investigating the spread of possibly infected saliva droplets between individuals during social contact, work, and transportation in common spaces. The fluid jets that possibly spread the saliva droplets are part of the flow from an individual's breathing and speech, in addition to coughing and sputtering from spasms. The jet is an aerodynamic structure rich in time and space scales that can travel long distances without dissipating, transporting what is contained in it Batchelor (2000); Panton (2013).

It is important to note that these aqueous particles suffer strong dynamic interference from the jet, resulting in unpredictable trajectories, in addition to eventually evaporating due to the intense exchange of heat and mass with the external environment. It is commonly agreed among researchers that effects such as drag, lift, evaporation and gravity are extremely important parameters for a complete evaluation of the trajectory of these particles, for example in Wells (1934) it is shown that the effects of inertia, surface tension and gravity are determinants in the duration of these particles, as well as the size of the drops after loss of mass by evaporation.

Similar to this research, Zhu S. (2006) studied the particle behaviour both experimentally and numerically with a CFD model of a flow inside a room. Zhaoa B. (2003) did the same, and found that the virtual mass and Basset forces are negligible under their experiment conditions, compared to buoyancy and drag. Xie X. (2007) simulates the evaporation rate of a single droplet, coupled with movement equations that represent drag, buoyancy and gravity. Liu L. (2016) developed a more complex evaporation model for the particle, where the particle composition is modeled by a fluid part composed of a sodium chloride solution and a insoluble solids part with an specific mass of $2000kg/m^3$, and it evaporates until it reaches an equilibrium diameter. Liu L. (2016) also works with drag and buoyancy forces, but inserts the particles in a turbulent jet.

To study the spread of possibly infectious saliva droplets, this research proposes simulating numerically the trajectory of saliva droplets expelled during conversation and coughing. A flow field in the Eulerian reference is described, with appropriate boundary conditions to simulate a jet in a designed region. In this flow field, particles are inserted in the jet region and their trajectory is described in the Lagrangian reference. The particles trajectory is recorded and plotted in a convenient manner.

Through the results of this numerical simulation, a better understanding about airborne disease transmission can be attained. By examining the data about how long the particles stay in the air, how they disperse, what distances they can reach and how long until they evaporate, better safety guidelines can be developed, especially for enclosed environments with poor ventilation.

The flow field is established utilizing a numerical solution for the Navier-Stokes equations for incompressible fluid. The droplets are represented by particles ruled by the Basset-Bousinesq-Ossen equations, and are designated to a location within the fluid flow where a jet is simulated. These particles are assigned an initial amount of momentum, which is then updated as their position changes.

This article is organized with an introduction of COVID-19/SARS-COV-2 models and the corresponding literature review, followed by the mathematical modeling used in this work including the 2-dimensional equations for fluid motion using the streamfunction-vorticity formulation and the Lagrangian tracking of particles. Next, the result section shows two important benchmarks cases fluid flow simulations, to assess and compare the accuracy of the proposed method, and two simulations with the particles, to analyse the saliva droplet behaviour. Finally, this text ends with remarks in the conclusion section.

2. METHODOLOGY

To describe the flow field, the Poisson equation, obtained from the Navier-Stokes equations as given by T. E. Tezduyar and Behr (1990), was numerically solved by the finite element method, using linear two dimensional triangular elements. The transport of vorticity ω_z, the Poisson equation for the streamfunction ψ and the recovery of the velocity field $\mathbf{v} = (v_x, v_y)$ are written as follows:

$$\frac{\partial \omega_z}{\partial t} + \mathbf{v} \cdot \nabla \omega_z = \frac{1}{Re} \nabla^2 \omega_z \tag{1}$$

$$\nabla^2 \psi + \omega = 0 \tag{2}$$

$$v_x = \frac{\partial \psi}{\partial y} \qquad v_y = -\frac{\partial \psi}{\partial x} \tag{3}$$

where ω_z is the z component of the vorticity field ω, t is time, $\mathbf{v}$ is the fluid velocity, Re is the Reynolds number as commonly defined in the literature, and ψ stands for the streamfuncion.

To simulate enclosed spaces, the mesh boundary conditions on what represented walls were set to respect the no slip condition, restricting the velocity in both horizontal and vertical directions.

To simulate the added jet of air when a person coughs or speaks, a small mesh area was finely discretized to simulate the mouth area, and velocity boundary conditions were set, based on values found by Soon-Bark Kwon (2012). Assuming a worst case scenario, the velocity boundary conditions were based on the values given by males, who Soon-Bark Kwon (2012) found, produce the highest coughing and speaking velocity values, at around 15.4m/s for coughing and 4.11m/s for speaking. The jet is not unidirectional however, and so the velocity values were distributed on an arc from $-17.9°$C to $19.9°$C, adjusting the x and y velocity values accordingly to the direction.

The size and number of saliva droplets that are expelled from the mouth when talking and coughing varies by wide range in the literature. While Soon-Bark Kwon (2012) finds the total number of particles expelled from one cough to be around one hundred, Loudon (1967) finds the same total to be around six thousand. Their size distribution is very similar, however, and the number utilized in this simulation follows the size distribution given by findings of C. Y. H. Chaoa (2008), with an estimated total number of 5000 particles total. The size distribution of those 5000 particles can be seen in table 1. The size class refers to an average size.

The saliva droplets are modeled as spheres, and the numerical simulation treats them as solid particles. Due to their small mass and volume, it's considered that the presence of the particles does not affect the fluid flow in any significant way. As stated in Loudon (1967) and Soon-Bark Kwon (2012), the particles evaporate, until they reach equilibrium and there's a smaller droplet nuclei left. These droplet nuclei can stay in the air for a long time.

According to Richard (2016), a particle trajectory is influenced by the forces between the fluid and the particle, forces imposed by external fields, and forces due to the interaction between particles. The modified Basset-Bousinesq-Ossen (BBO) equation is utilized to simulate those forces, as they're applied to each particle, and is given by:

$$\frac{d\mathbf{u_P}}{dt} = \frac{3C_D\rho}{4d_p\rho_p}|\mathbf{u} - \mathbf{u_P}|(\mathbf{u} - \mathbf{u_P}) + \frac{1\rho}{2\rho_p}C_I\frac{d}{dt}(\mathbf{u} - \mathbf{u_P}) + \frac{\rho}{\rho_p}\frac{D\mathbf{u}}{Dt}$$
$$+ \frac{9\rho}{d_p\rho_p}\left(\frac{\nu}{\pi}\right)^{1/2}C_B\int_{t_0}^{t}\frac{d/d\tau(\mathbf{u} - \mathbf{u_P})}{\sqrt{t - \tau}}d\tau + \left(\frac{\rho}{\rho_p} - 1\right)\mathbf{g}. \tag{4}$$

Table 1. Particle size distribution when an individual speaks and coughs.

Particle size class μm	Speaking	Coughing
3	2,8%	3,6%
6	44,3%	49,9%
12	15,2%	18,5%
20	7,9%	6,1%
28	5,3%	2,3%
36	2,6%	2,2%
45	2,8%	1,8%
62.5	3,0%	1,8%
87.5	2,1%	1,3%
112.5	2,8%	1,5%
137.5	2,6%	1,4%
175	2,8%	4,0%
225	2,5%	2,3%
375	2,3%	1,9%
750	0,8%	1,3%
1500	0,0%	0,0%

where $\mathbf{u_p}$ is the particle's velocity vector, $\mathbf{u}$ the fluid's velocity field, ρ_p is the particle's density, ρ is the fluid's density, ν is the fluid's kinematic viscosity, d is the particles diameter.

C_D, C_I and C_B are drag, the virtual mass and Basset coefficients, respectively. Those are given, as described in D. Hansell and Kollmann. (1992), by:

$$C_D = \frac{24}{Re}\left(1 + \frac{Re^{\frac{2}{3}}}{6}\right) \qquad\qquad Re < 1000 \qquad\qquad (5)$$

$$C_I = 2.1 - \frac{0.132A_n^2}{(1 + 0.12A_n^2)} \qquad\qquad Re < 62 \qquad\qquad (6)$$

$$C_B = 0.48 + \frac{0.52A_n^3}{(1 + A_n^3)} \qquad\qquad Re < 62 \qquad\qquad (7)$$

where Re and A_n are the Reynolds number and the acceleration number respectively, defined according to the following expressions:

$$Re = \frac{|\mathbf{v} - \mathbf{u_p}|d}{\nu} \qquad\qquad (8)$$

$$A_n = \frac{|\frac{d(\mathbf{v} - \mathbf{u_p})}{dt_p}|}{|\mathbf{v} - \mathbf{u_p}|^2}d \qquad\qquad (9)$$

As the particles move through the air, they lose mass to evaporation. This has the effect of reducing the particle's diameter over time, which directly impacts the drag forces acting on the particle. Deduced from Fick's law, an equation to account for the diameter reduction is found on Crowe C. T. (2012), and is given by:

$$d^2 = d_o^2 - \lambda t \qquad\qquad (10)$$

$$\lambda = \frac{4Sh\rho D_v}{\rho_p}(\omega_{A,s} - \omega_{A,\infty}) \qquad\qquad (11)$$

where d_o is the particle's initial diameter, Sh is the Sherwood number, D_v is the diffusion coefficient, $\omega_{A,s}$ is the mass fraction of water at the particle's surface, and $\omega_{A,\infty}$ is the mass fraction of water in the atmosphere.

On this research, the saliva was modeled as a solid particle, however when a collision between particles happen, it's considered the particles participant on the collision coalesce into a single particle, with mass and momentum given by

$$m_1 + m_2 = m_{1+2} \qquad \text{and} \qquad P_1 + P_2 = P_{1+2} \qquad\qquad (12)$$
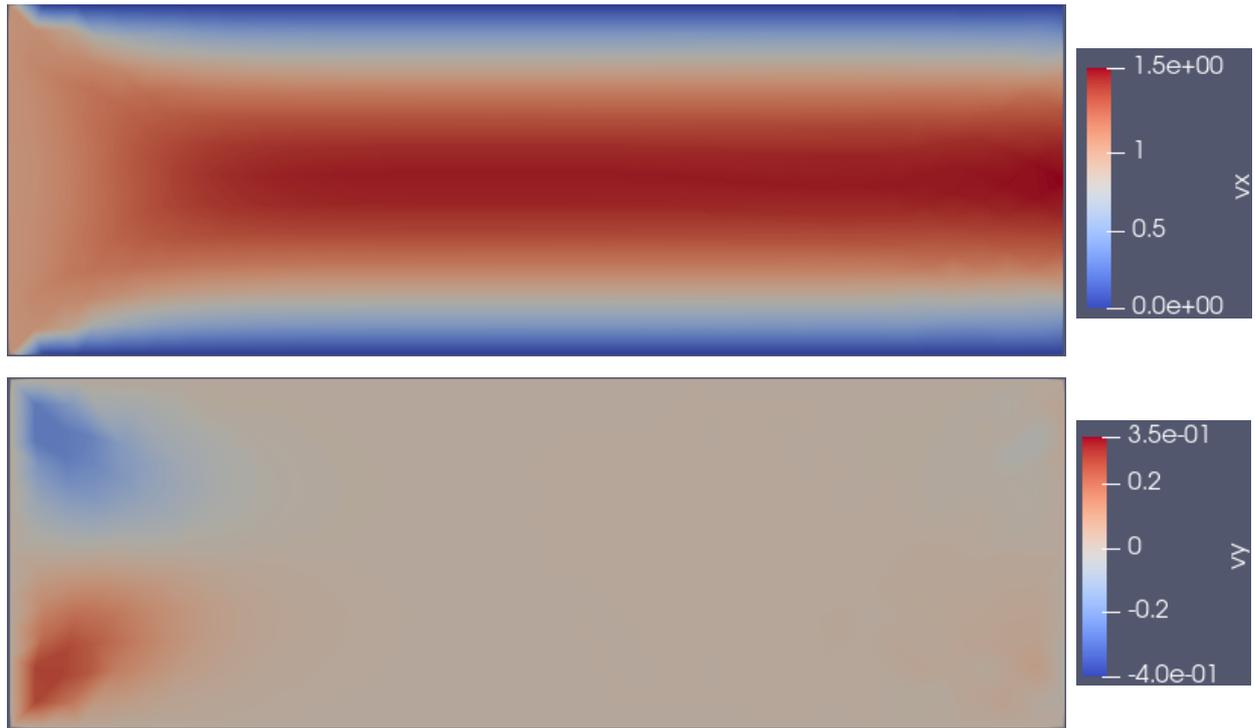
Figure 1. 2-dimension Hagen-Poiseuille solution for horizontal v_x and vertical v_y velocities using the streamfunction-vorticity formulation.

respectively, with m representing the particle mass and P the particle's momentum. Additionally, collisions between a saliva particle and a wall or obstacle result in the saliva droplet adhering to said wall. On such an occasion then, the numerical simulation sets the colliding particle momentum to zero, fixing it in place, and prevents the momentum value from being changed in future iterations, essentially fixing the particle in space.

The numerical code has been hand crafted using state-of-the art technique with Finite Element Method to discretize the fluid equations. The convective term, source of undesired spurious instabilities has been modeled using the Semi-Lagrangian method which is unconditionally stable even for high Reynolds numbers and high time steps dt (Anjos *et al.* (2020)). The solution of the numerical algorithm is made on an unstructured triangle mesh generated by Gmsh (Geuzaine and Remacle (2009)) with refined zones next to the region of interest. The Conjugated Gradient solver with the incomplete Cholesky preconditioner has been used as solution for the linear systems resulting from the discretization of the vorticity transport equation, the streamfuncion equation and the computation of the velocity field.

3. RESULTS

3.1 Validation: Hagen Poiseuille flow and Lid-Driven Cavity for moderate Reynolds numbers

In figures 1 and 5, one can observe the numerical solution for the velocity fields of two important benchmarks in fluid dynamics namely Hagen-Poiseuille and Lid-Driven cavity flows, respectively. Good accuracy was found at both simulation where the chosen parameters were $Re = 10$ with Δt intervals of 0.01s, for 200 iterations. Both simulation's meshes used 2-dimensional linear triangular elements. The Hagen-Poiseuille simulation was realized using 417 nodes and 1046 elements and the Lid-Driven cavity flow used 142 nodes and 406 elements.

Despite the low Reynolds numbers, the current code is ready to simulate laminar to turbulent flows with accuracy. The numerical results obtained for the Hagen-Poiseuille example are almost exactly the same as it's analytical solution. As for the Lid Driven cavity example, the simulation results in the expected spatial behaviour.

3.2 COVID-19 jet stream with random distribution of droplets

Two similar simulations were elaborated, both using the same finite element mesh elaborated to resemble a face profile, composed of 2-dimensional linear triangular elements, with 2354 nodes and 5122 elements. The boundary conditions and dimensions for the mesh utilized for the fluid flow simulations can be observed in 3. In **??**, one can see the mesh detail close to the face profile.

The reference velocities used for the speech and cough examples are respectively 4.11 m/s and 15.4 m/s. The reference
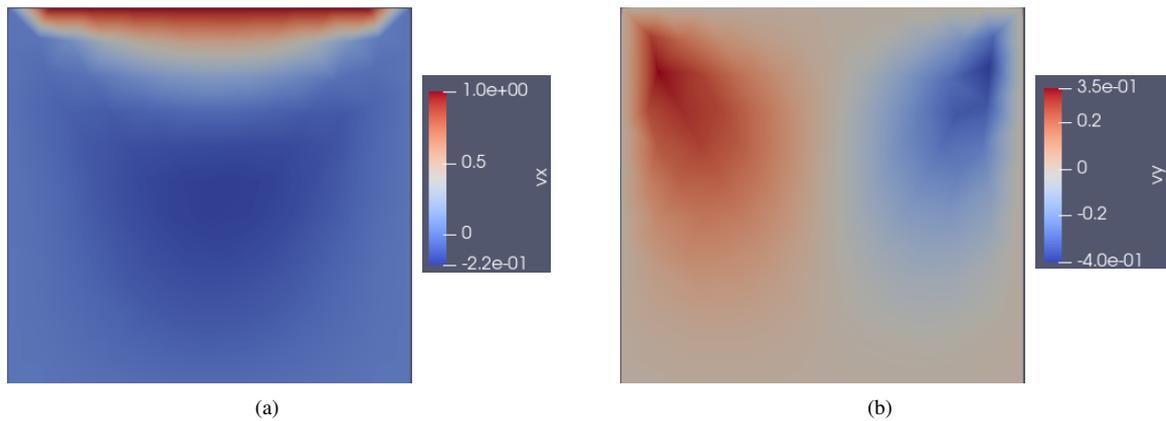
(a)   (b)

Figure 2. 2-dimensional Lid-Driven Cavity solution for horizontal v_x and vertical v_y velocities using the streamfunction-vorticity Finite Element formulation. Results are in qualitative agreement with literature.

length for both simulations is $0.01m$, and air specific mass and viscosity of 1.204kg/m³ and 1000kg/m³. The resulting Reynolds number for the speech example was 2719 and for the cough example 10188, and both simulations were run with Δt intervals of 0.035s, for 570 iterations. The cough jet was simulated as continuous, which is a good approximation for the short time frame of the simulation.

Over the face profile mouth region, non-dimensional horizontal velocity boundary conditions of 1 were assigned, while values of 0 were assigned to the rest of the control volume's boundary.
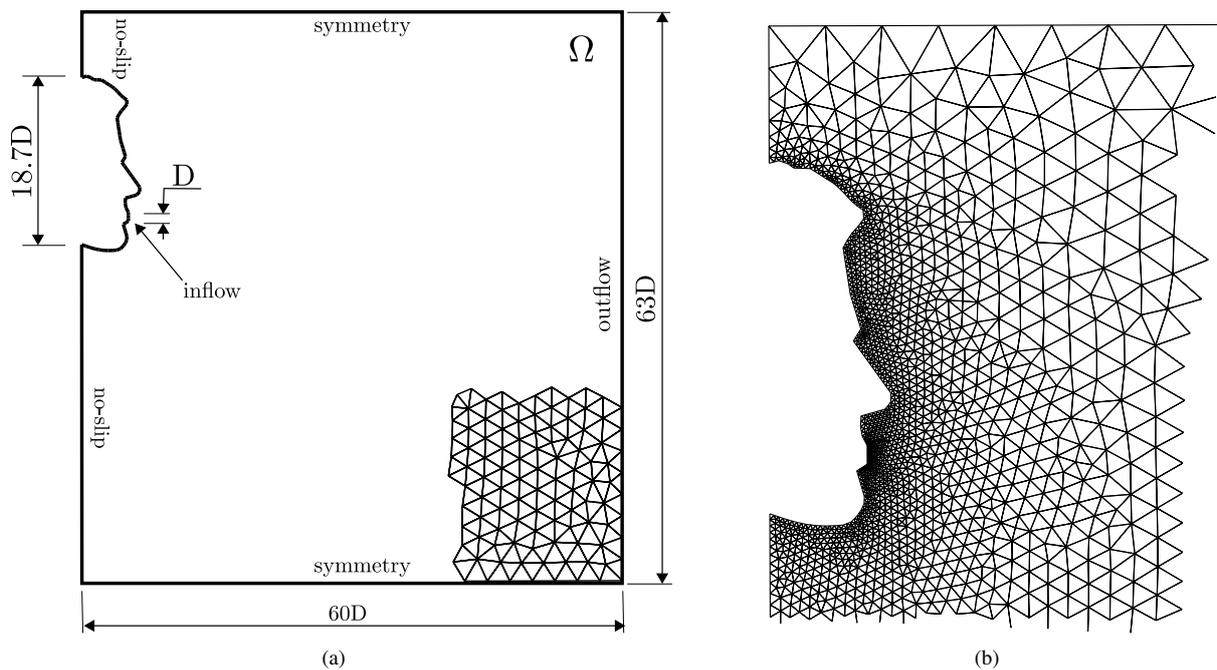

(a)   (b)

Figure 3. Detailed schematic diagram of the air jet stream with droplets simulation. (a) The geometry was built from a standard human face resulted as image post processing. The dimensionless mouth was set to $D = 1$ while all the others dimensions were set accordingly. (b) Detailed view of the unstructured triangle finite element mesh close to the human profile. It can be noted that higher mesh refinement was used to accurately describe the flow dynamics from the mouth.

In both simulations, 5000 particles were assigned to a region close to the face profile's mouth. Those particles were randomly assigned a diameter, using the distribution for speech and cough displayed on table 1, and an initial velocity of 4.11m/s and 15.4m/s respectively. The velocity direction was not horizontal, and instead randomly assigned an angle between $-17.9°C$ to $19.9°C$, to simulate the natural particle dispersion observed by Soon-Bark Kwon (2012). The particles were simulated as spheres composed of pure water, with an specific mass of 1000kg/m³, inserted in an air flow with specific mass of 1.204kg/m³, with a 60% humidity. For this simulation only the drag, buoyancy and gravity terms of the BBO equation were utilized.
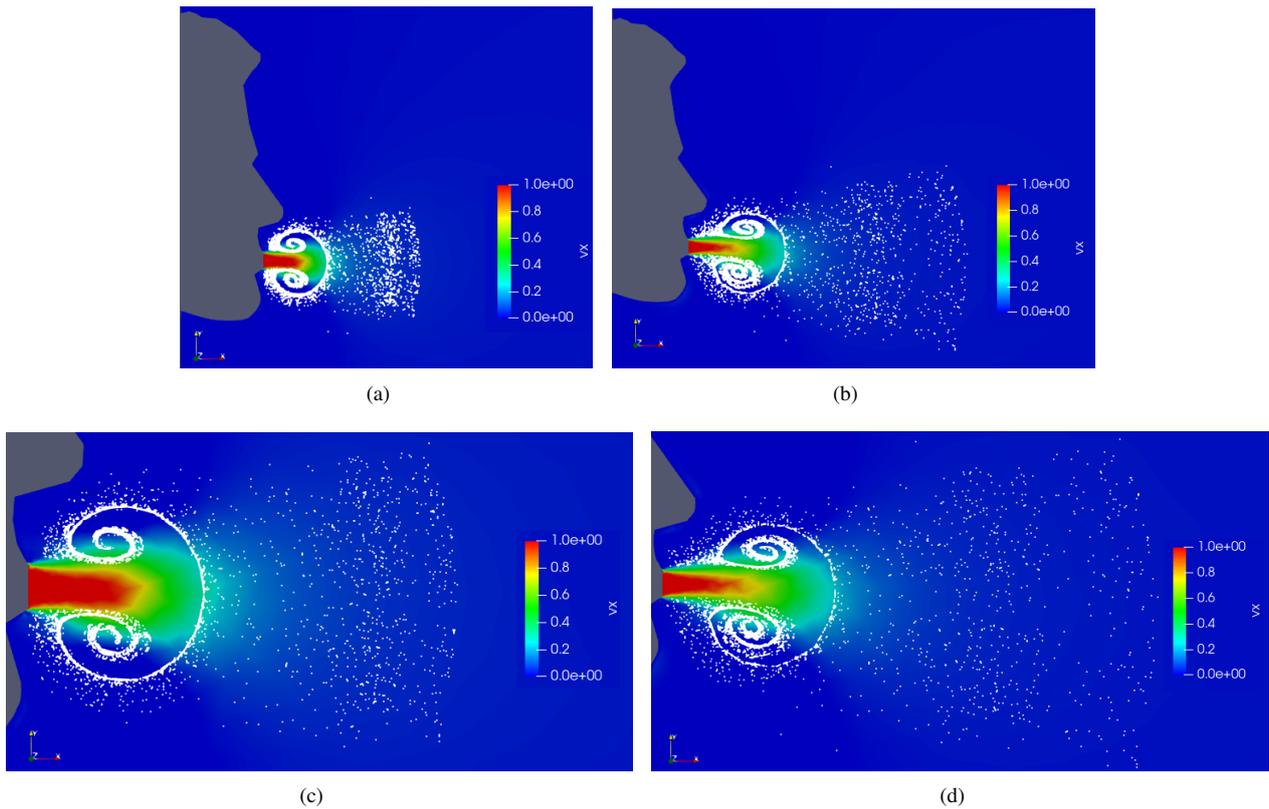
Figure 4. 2-dimensional jet stream simulation for a person's speech with using the streamfunction-vorticity Finite Element formulation, coupled with 5000 particles based on the BBO equation. Figures a and b represent iterations 285 and 570, of the simulation progress with the face profile, and Figures c and d represent the same iterations with a close-up

4. CONCLUSION

From the simulation's results, one can observe the particles interaction with the fluid flow around them. The heavier particles, despite their biggest diameter, were less affected by the drag forces, and were just slowed down on their trajectory. The smaller, more numerous particles, were caught by the vortexes on the upper and lower regions of the jet, swirling in place, and staying close to the face profile. This result is expected, because mass grows exponentially with radius, and a heavier particle carries considerably more momentum. One can also observe, in the small time frame of the simulation, that gravity effect's is close to negligible. The heavier particles tended to maintain their linear trajectory, while there is little sign that gravity affected the smaller particles closer to the face profile and trapped inside the vortexes.

5. LIMITATIONS

Saliva particles are composed of water and a smaller, particle nuclei, composed of solid matter. In the simulation, the particles were represented as if composed entirely of water. This impacts on the accuracy of the evaporation rates, specially when simulating long periods of time, and on the particle's specific mass values.

People in enclosed spaces, such as supermarket lines, malls, living rooms, etc, often move, and such movement disturbs the flow field, in a way that is not simulated in this article. Obstacles in the particles trajectory, such as furniture, product stands in stores, and even other people also influence the fluid flow, but being of complex and of 3-dimensional shape, demand a much more detailed 3-dimensional simulation.

6. FURTHER DEVELOPMENT

While the most important term of the BBO equation is the drag term, the virtual mass and Basset terms might have a significant impact on the simulation's accuracy, and including them might offer improved results.

Another factor that might impact accuracy is modeling the particle by water surrounding a solid particle nuclei. Depending on how much the droplet nuclei's specific mass differs from water's, a change might be observed compared to the current simulation.

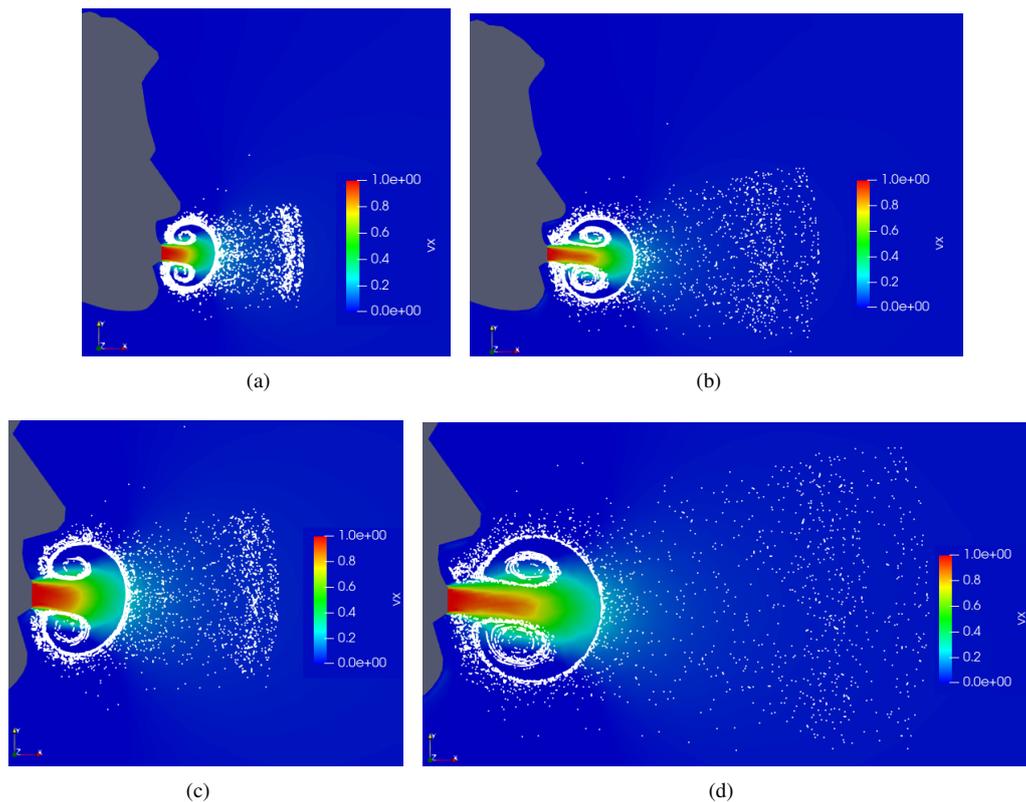We aim to consider such factors in future simulations and new results will be presented.

Figure 5. 2-dimensional jet stream simulation for a person's speech with using the streamfunction-vorticity Finite Element formulation, coupled with 5000 particles based on the BBO equation. Figures a and b represent iterations 285 and 570, of the simulation progress with the face profile, and Figures c and d represent the same iterations with a close-up

7. ACKNOWLEDGEMENTS

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