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Bachelor Project

Applied Mathematics

Analysis of the 1.5m Social Distance Restriction by the Simulation of Flying Water Droplets

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Abstract

To stop the spread of COVID-19 during the current pandemic, several measures such as the social distance restriction have been implemented. However, the magnitude of the restriction differs per country. In this study, the social restriction measure is being investigated from a mathematical perspective. A 2-phase simulation is set up in ComFLOW to investigate the horizontal displacement of a water droplet from a person's mouth or nose to the ground. To verify the results from ComFLOW, first an ODE model is derived. The results of this model are generated with the use of MATLAB. When the maximum velocity was considered, this resulted in a required social distance of 1.32 meter. To achieve a credible model, several attempts have been made in ComFLOW. In the final attempt, the droplet starts in a tube, which is made of ellipses and rectangles to create a positive horizontal velocity with the use of gravity. The simulations in ComFLOW show that the simulation of a small droplet is not computationally efficient and causes the droplet to spray out. Increasing the viscosity of the water is beneficial for the simulation, yet it causes a longer computational time. In conclusion, ComFLOW is a not an ideal program for simulating a flying water droplet.

Contents

Chapter 1

Introduction

For more than one year, the coronavirus has been part of our lives. The disease COVID-19 is caused by the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). Since the virus first emerged in China in December 2019, it has spread to nearly every country in the world [1]. To fight the virus, many countries have implemented social distancing as one of the safety measures. However, the magnitude of social distancing differs throughout the world. For example, in The Netherlands the guideline is 1.5 meters, in Spain 2 meters and in Austria 1 meter [2–4].

The scientific origin of the measure to keep a distance of 1-2 meters can be traced back to a study from 1942, among others [5]. However, this study and others in which the evidence for the 1-2 meter measure is given have been criticised by other researches [6, 7]. Therefore, in this Bachelor Thesis the social distance restriction will be investigated from a mathematical perspective.

The aim of this research is to set up a 2-dimensional model in ComFLOW to simulate the motion of a mucus droplet from a person's mouth or nose to the ground. Due to the fact that a mucus droplet consists mainly of water, a water droplet will be simulated [8]. ComFLOW is a program for the numerical solution of fluid, based on the Navier-Stokes equations [9]. In this study, it has to be investigated whether ComFLOW is the appropriate program for this simulation. Eventually, with the use of simulations, advise can be given on the credibility of the current measures. It can also be analyzed which countries have chosen the "best" social restriction.

The structure of this Bachelor thesis is as follows. In Chapter 2, the evidence on the distance measures and the spreading of the coronavirus is discussed. In Chapter 3, a simplified ODE model of the motion of a water droplet is derived. The solution of this model, which is achieved with the use of MATLAB, will be used to verify the results from ComFLOW. In Chapter 4, the mathematics and numerics behind ComFLOW and the results of the ComFLOW simulations will be shown. Moreover, several attempts which eventually lead to the preferred simulation of the water droplet will be outlined. In Chapter 5, the conclusion and summary of the research will be given. Furthermore, the reliability and applicability of the research will be discussed. In the Appendices, the input files from the results obtained in MATLAB and ComFLOW can be found.

Chapter 2

Literature research

All over the world, health organisations give recommendations regarding the best strategies in the battle against the coronavirus. However, the recommendation these institutes provide are not fully inline with each other. The World Health Organisation (WHO) has issued guidelines for contact and droplet precautions on international level. They advise among other things to maintain at least one meter of social distance [10]. On European level the European Centre for Disease Prevention and Control (ECDC) advises maintaining a physical distance of ideally two metres [11]. In The Netherlands, the "Rijksinstituut voor Volksgezondheid en Milieu" (RIVM) has the advising role for the measures in the battle against corona. They advise to maintain a social distance of 1.5 meters. In this Chapter, it is investigated on which this 1-2 meter range of social distance is based. Secondly, it is discussed why The Netherlands has chosen the 1.5 meters measure. Thirdly, it is investigated how the coronavirus can spread.

2.1 Evidence of the distance measures

The scientific origin of the measure to keep a distance of 1-2 meters can be traced back to, among others, a study from 1942. In this study, it was shown that the majority of the larger droplets traveled a horizontal distance of less than 1 meter using photo technology [5]. This research was later criticized. The used technique is not suitable for photographing all droplets. Besides, the arrangement was such that droplets that traveled more than 2 meters were not even recorded. Moreover, the study did not take into account the influence of air currents [6].

Recently, Australian researchers have compared ten studies. These studies looked at the distance larger droplets can travel horizontally, when someone sneezes or coughs, in a lab setup. This research has proven that in eight of the ten studies, larger droplets were able to travel a horizontal distance larger than 2 meters. Some studies even show a distance of six to eight meters. The researchers conclude that the current measure of 1 to 2 meters of physical distance is not scientifically substantiated. Furthermore, the researchers state that the horizontal distance that droplets can travel is influenced by many factors. These factors include temperature, humidity, ventilation, exhalation rate and evaporation rate, which makes it difficult to determine an adequate distance measure [7]. A shortcoming of this study is that the researchers did not check whether such droplets would contain enough virus particles to be contagious [6].

Furthermore, a group of Canadian researchers has recently released a study in the Lancet. In this study, they bring together and analyze the findings of a large number of studies on the effects of some well-known measures, such as physical distance and face masks. Based on a comparison of 172 observational studies on the transmission of COVID-19, SARS and MERS, the researchers conclude that at least 1 meter of physical distance is associated with a reduction in the risk of infection. They calculated that the probability of becoming infected at less than 1 meter physical distance is 13%, against 3% when more than 1 meter physical distance is kept. The researchers therefore conclude that there is a scientific basis for keeping a physical distance of 1 meter or more [12]. On the website of the RIVM they explicitly refer to this study to substantiate the 1.5 meter measure [2].

However, the Canadian study is not uncontroversial. Firstly, it appears that in some cases the underlying data is of low quality or has not been subjected to an independent scientific assessment. For example, due to the fact that the risk of biases is high and the use of peer reviews [13]. Secondly, a re-analysis of the study shows that the dataset may have been misinterpreted and that 80% of the positive effect of physical distance already occurs when keeping less than 1 meter social distance [14]. Thirdly, several studies have tried to replicate the Canadian study. However, these studies proved that the results were based on (unsubstantiated) assumptions about physical distance used in the meta-analysis in the studies [15].

Researchers from the Center for Evidence-Based Medicine affiliated at the University of Oxford have investigated the extent to which 2 meters of physical distance is adequate to limit transmission of the coronavirus [16]. To answer this question, the researchers used 120 studies that have already been conducted into the spread of the coronavirus in various environments, such as households, restaurants, cruise ships and hospitals. An important finding is that it is difficult to conclude on the effect of physical distance, due to the fact that the studies are heterogeneous. Therefore, it is difficult to compare these studies with each other. Another finding is that long-term exposure in a confined space can be linked to "hotspots" with contamination, such as choirs, sporting events and fitness centers. Note that within this finding, the information about the physical distance between people is unknown. The researchers conclude that keeping a physical distance is associated with a lower risk of infection. However, at the same time they state:

"Single thresholds for social distancing, such as the current 2-metre rule, oversimplify what is a complex transmission risk that is multi factorial. Social distancing is not a magic bullet to eliminate risk. A graded approach to physical distancing that reflects the individual setting, the indoor space and air condition, and other protective factors may be the best approach to reduce risk" [16].

A British study shows that the chance of becoming infected with the coronavirus in an indoor space depends on many factors. Thus, this study resonates in studies by other authors [17–20]. Factors that are often mentioned are aerosol properties, indoor air flow, ventilation, type of activity, virus specific characteristics and specific characteristics of the people inside (i.e., the degree to which people inside are susceptible to the virus) [19].

An important comment must be made in the discussion of the scientific literature so far. It should be noted that the findings and conclusions from the British research mainly relate to studies looking at (the effects of) physical distance in indoor spaces. It is not yet known to what extent keeping a physical distance helps to limit virus transmission in outdoor conditions [21].

2.2 Spreading of coronavirus

People may get get infected with the coronavirus through close contact with a person who has symptoms from the virus. It is generally spread via airborne mucus droplets, which originate from coughing and sneezing [22]. Mucus is for 98 percent composed of water, the other 2 percent consists of epithelial (surface) cells, dead leukocytes, mucin, and inorganic salts [8, 23]. Therefore, in this research an airborne water droplet released from sneezing or coughing is simulated to see how far such a droplet will travel and whether the measures are sufficient to reduce the infection rate. To get a reliable model, it will be investigated what happens when a person sneezes or coughs and what velocities a mucus droplet reaches during these activities.

Firstly, the effect of sneezing is investigated. As discussed in [24], sneezing is a way of removing irritants from your nose or throat. The sneezing reflex can be divided into two phases. The first phase is the nasal or sensitive phase, following stimulation of the nasal mucosa by chemical or physical irritants. After reaching a threshold, the second phase will start, which consists of eye closing, deep inspiration, and then a forced expiration with the initial closing of the glottis, and increasing intrapulmonary pressure. The glottis is the opening between the vocal folds [25]. Besides, the intrapulmonary pressure is the pressure between the pleura, which is a thin layer of tissue that covers the lungs and lines the interior wall of the chest cavity [26]. The sudden dilatation of the glottis gives rise to an explosive exit of air through the mouth and nose, washing out mucosal debris and irritants [24]. The velocity of such a sneeze is approximately 50.0 m/s [27].

Secondly, coughing will be looked into. As discussed in [28], a cough is a natural defense mechanism that protects the respiratory tract from inhaling foreign bodies. In addition, coughing clears excessive bronchial secretions. Coughing can be divided into four phases. First, the receptorial phase, which simulates the cough receptors and sends an impulse to the center. Second, the inspiratory phase, which consists of opening the glottis with rapid inhalation. Third, the compressive phase, which consists of a prompt closure of the glottis with consequent adduction of the vocal cords. At the same time, there is a strong contraction of the abdominal muscles and other expiratory muscles resulting in increased intrapulmonary pressure and compression of the alveoli and bronchioles. The final phase is the expiratory phase, in which the vocal cords and epiglottis suddenly open. This causes the explosive leakage of air from the lungs to the outside. Subsequently, the exhalation continues, favored by the complete relaxation of the diaphragm. The velocity of a cough is approximately 10 m/s [27].

Chapter 3

Mathematical ODE model

To gain better insight into how a water droplet moves through the air, from the mouth or nose to the ground, a mathematical model will be derived. In this model, the forces acting on the droplet will be evaluated to obtain a relation between the air density, the volume of the droplet, height of the mouth and the distance the droplet travels.

The motion of the droplet is assumed to behave as shown in Figure 3.1. At each time in the motion of the droplet, the velocity of the droplet can be decomposed in the x- and y-direction. This is shown in Figure 3.1 at three different points.

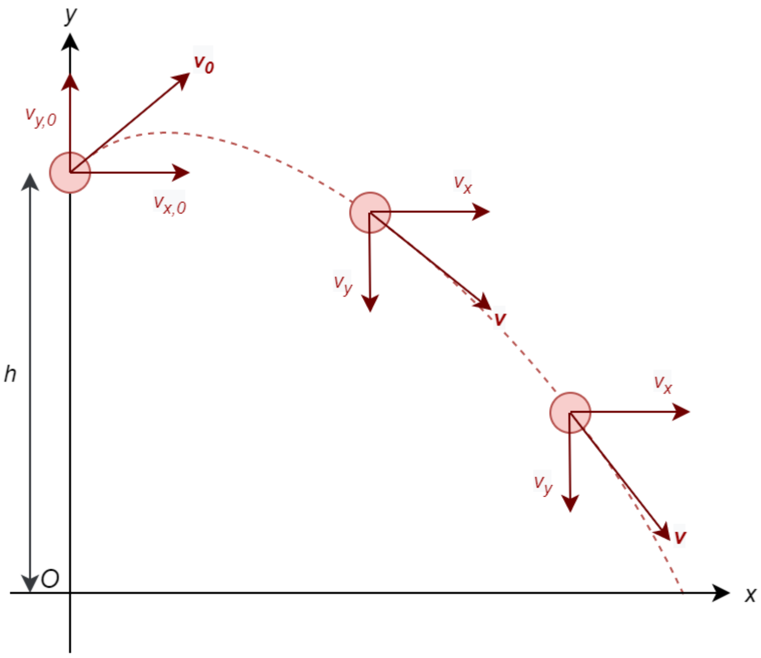


Figure 3.1: Vector decomposition of a moving droplet.

In Figure 3.1, the h represents the initial height. $\mathbf{v_0}$ is the initial velocity vector, which is decomposed into its components, $v_{x,0}$ and $v_{y,0}$, in the x- and y- direction, respectively. Furthermore, at each point in the motion of the droplet the velocity vector $\mathbf{v}$ is decomposed into v_x and v_y. Therefore, the magnitude of the velocity is given by

$$||\mathbf{v}|| = \sqrt{v_x^2 + v_y^2} \tag{3.1}$$

In this chapter, it is assumed that the droplet that comes out of a person's mouth from a certain height, h, only has an initial horizontal velocity. As a result $v_{y,0} = 0$ and $v_{x,0}$ will be equal to the velocity the droplet has when it comes out of a person's mouth, which is in the range from 10 to 50 m/s [27].

3.1 Motion of the droplet without air resistance

First, the motion of the water droplet without air resistance will be investigated. In this case, the only force acting on the droplet with mass m is the gravity in the y-direction. By Newton's second law [29], the following can be obtained for the forces acting on the droplet in two directions:

$$\begin{aligned} m \cdot a_x &= \sum F_x = 0 \\ m \cdot a_y &= \sum F_y = -F_z = -m \cdot g. \end{aligned}$$

Thus, the components of the acceleration of the droplet are

$$a_x = 0 \quad \text{and} \quad a_y = -g,$$

where g is the gravitational acceleration [30]. Due to the fact that the acceleration is constant, the landing point of the droplet can be easily calculated. For this, the relation between distance, x, velocity, v, and acceleration, a, can be represented as

$$a(t) = \frac{dv}{dt}(t) = \frac{d^2x}{dt^2}(t).$$

Consequently, the general equation for an initial distance x_0, velocity v_0 and constant acceleration a is

$$\begin{aligned} a(t) &= a \\ v(t) &= v_0 + at \\ x(t) &= x_0 + v_0 t + \frac{1}{2}at^2 \quad [29]. \end{aligned}$$

In this research, when assuming that the initial velocity in the y-direction is zero and in the x-direction is equal to v_{start}, the following relation for x and y can be obtained

$$\begin{aligned} x(t) &= v_{start} t \\ y(t) &= h - \frac{1}{2}gt^2. \end{aligned}$$

Eliminating t will give the following parabolic relation between x and y

$$y(x) = h - \frac{g}{2v_{start}^2}x^2.$$

Hence, the trajectory of the droplet has a quadratic relation, which is in line with what was drawn in Figure 3.1. Furthermore, by solving $y(x) = 0$, it can be seen that the droplet reaches the ground at $x_{ground} = \sqrt{\frac{2hv_{start}^2}{g}}$. In conclusion, for the analytical model without air resistance, the droplet travels x_{ground} meters horizontally.

3.2 Motion of the droplet with air resistance

Next, the motion of the droplet, when the air resistance is included, will be investigated. The standard formula for air resistance is

$$F_w = \frac{1}{2}\rho C_d A v^2, \tag{3.2}$$

where, ρ, C_d, A are the density of the air, the drag coefficient and the cross sectional area of the droplet, respectively [29]. For readability, the form $F_w = kv^2$, with $k = \frac{1}{2}\rho C_d A$ will be used from now on. Since a velocity vector is considered, the air resistance force will have the following form

$$\mathbf{F_w} = k||\mathbf{v}||\mathbf{v},$$

where the magnitude, $||\mathbf{v}||$, is defined as in (3.1). Subsequently, for both components the following force can be obtained

$$\begin{aligned} F_{w,x} &= k||\mathbf{v}||v_x \\ F_{w,y} &= k||\mathbf{v}||v_y. \end{aligned}$$

Thus, the air resistance has to be included into the summation of the forces in both components. By using Newton's second law, the following equation can be obtained

$$\begin{aligned} m \cdot a_x &= \sum F_x = -F_{w,x} = -k||\mathbf{v}||v_x \\ m \cdot a_y &= \sum F_y = -F_z - F_{w,y} = -mg - k||\mathbf{v}||v_y. \end{aligned}$$

As a result, the components of the acceleration of the droplet are

$$a_x = -\frac{kv_x}{m}||\mathbf{v}|| \quad \text{and} \quad a_y = -g - \frac{kv_y}{m}||\mathbf{v}|| \quad [30].$$

As can be seen, there are no constant acceleration components anymore. Consequently, a numerical solution method is needed to obtain the solution for the travelled horizontal distance of the droplet.

3.2.1 Numerical solution

To find a numerical result for the model with air resistance, the Forward Euler method will be used twice. The Forward Euler method is a first order numerical solution procedure for ordinary differential equations with a given initial value. [31].

Since a mucus droplet consists of 98 percent of water [8], it is assumed to have a spherical water droplet. Furthermore, some other assumptions are made and several parameters are used, which can be found in Table 3.1.

Quantity	Given value
Area of the droplet	$A = 1.0$ mm^2
Volume of the droplet	V =1.0 mm^3
Density of the droplet	$\rho_d = 997$ kg/m^3 [30]
Density of the air	$\rho_a = 1.2041$ kg/m^3 [30]
Gravity force constant	$g = 9.81$ m/s^2 [30]
Temperature of the medium	$T = 20\ °C$
Drag coefficient	$C_d = 0.47$ [32]
Initial velocity	$v_{start} = 50$ m/s [27]
Initial height	$h = 1.75$ m

Table 3.1: Parameters for the motion of the droplet

With these parameters, the MATLAB script, which can be found in Appendix A.2.1, gave the following motion for the droplet.

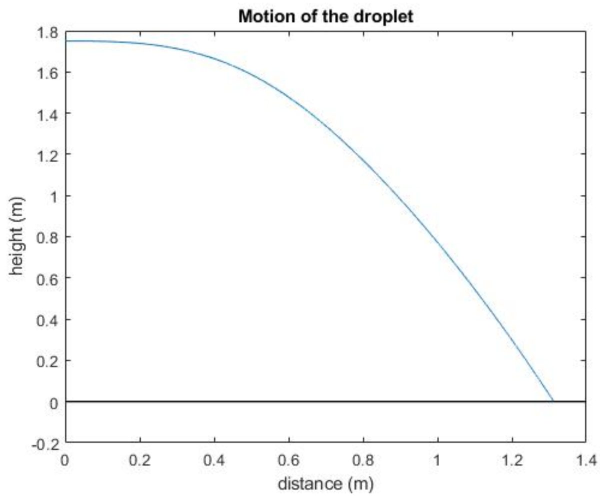


Figure 3.2: Motion of the droplet with air resistance.

As can be seen in this figure, the droplet moves similarly to the trajectory in Figure 3.1 and travels precisely 1.3231 meters horizontally from the mouth. This is within the range of 1 to 2 meters, which the health organisations advise as measure against the coronavirus. When including the solution without the air resistance with the same initial data, the following Figure is obtained, using the MATLAB script in Appendix A.2.2.

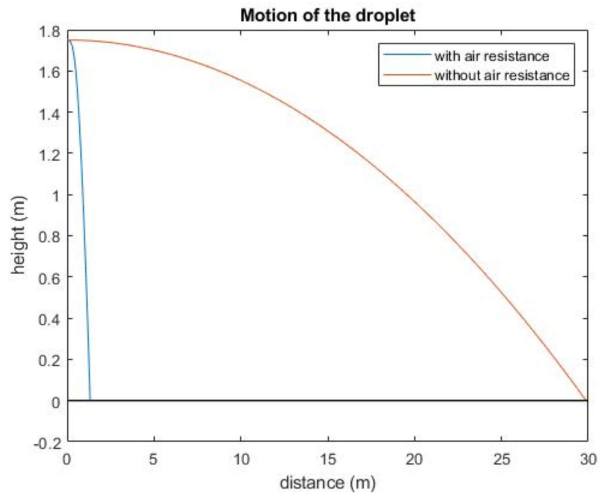
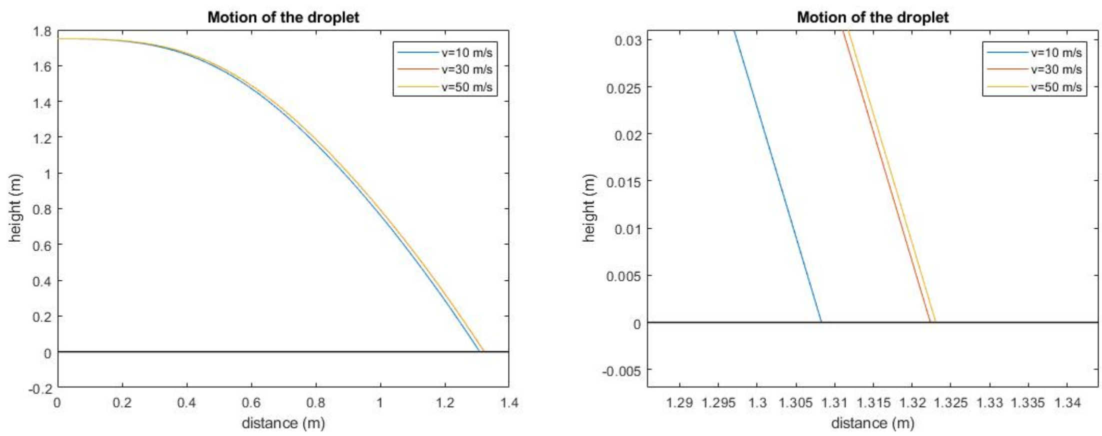


Figure 3.3: Motion of the droplet with and without air resistance.

Figure 3.3 shows that the droplet will have a far larger horizontal movement when there is no air resistance. Thus, the influence of the air resistance plays a significant role in the distance the mucus droplet travels. Therefore, in the ComFLOW simulation a two-phase approach is followed. A two-phase simulation is a numerical computation in which two fluids are considered [33]. In the case of the flying droplet, both water and air will be considered as moving fluids.

Furthermore, the influence of the starting velocity on the horizontal displacement is investigated. As can be seen in Table 3.1, the maximal sneezing velocity is used to obtain the results above. In Figure 3.4, also some other velocities in the range between the velocity of couching (10 m/s) and sneezing (50 m/s) are simulated. These results are obtained using the script in Appendix A.2.3.



(a) Result

(b) Zoomed in version of a

Figure 3.4: Motion of the droplet with different starting velocities.

Figure 3.4b shows that the difference between the horizontal displacement during coughing and sneezing is approximately 1.5 cm. Furthermore, the higher the starting velocity, the less influence this velocity will have on the additional horizontal displacement.

Chapter 4

ComFLOW

Several forces are acting on the water droplet during its trajectory. Since in the previous chapter only the air resistance and the gravitational force were considered, the program ComFLOW is used in order to obtain a more reliable model of the movement of the water droplet from a person's mouth or nose to the ground. ComFLOW is a program for the numerical simulation of fluid flow, based on the Navier-Stokes equations [9]. ComFLOW is normally used as a numerical tool for marine and offshore industries to study complex free-surface problems such as water waves around ships and platforms. Therefore, the input data has to be adjusted to simulate the movement of the water droplet. Besides, it has to be investigated whether ComFLOW is an appropriate program for such a simulation.

In this chapter the mathematics and numerics behind ComFLOW is discussed shortly. Subsequently, the attempts which lead to the simulation of a flying water droplet are discussed. For a broader explanation of the program, the user Manual ComFLOW version 3.9.X / 4.0 can be referenced [9]. For the post-processing of the data the Manual for the ComFLOW pre-post-processor [34] can be read.

4.1 Mathematics and numerics

In this section, a short introduction to the mathematical and numerical model on which ComFLOW is based is given. More detailed information is given in [9].

4.1.1 Mathematical model

In this research a two-phase flow is considered. For a two-phase flow model, considering water as an incompressible viscous fluid and air as a compressible viscous fluid, the Navier-Stokes equations are given by:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \qquad \textit{conservation of mass}$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla p + \nabla \cdot (\mu \nabla \mathbf{u}) + \rho \mathbf{F} = 0 \qquad \textit{conservation of motion.}$$

Where $\mathbf{u} = (u, v, w)$ stands for the velocity vector, ρ for the density, μ for the dynamic viscosity, p for the pressure and $\mathbf{F}$ stands for the external forces. A relation between the pressure and the density is required to close the system of equations. This relation is only applied to the compressible parts of the flow, namely the air. The adiabatic equation of state is used:

$$\frac{p_g}{p_{ref}} = \left(\frac{\rho_g}{\rho_{ref}}\right)^{\gamma} \tag{4.1}$$

Where p_g and ρ_g represents the pressure and density values of the compressible gas, respectively, and γ stands for the adiabatic coefficient. The reference values p_{ref} and ρ_{ref} can be specified in the input-file, `comflow.in`.

As discussed in [9] only boundary conditions are needed at domain boundaries and not at the free surface due to the fact that a two-phase flow is considered. At solid boundaries and objects, it is demanded that no fluid can go through the boundary and that the fluid "sticks to" the wall because of the viscosity. This is represented in the formula $\mathbf{u} = 0$ which is imposed at the solid boundaries of the domain and at solid objects. Capillary forces describing the interaction between gas and liquid are included in $\mathbf{F}$ and are imposed at the free surface.

In grid cells at the liquid-gas interface, the density and viscosity in the cell centres can be calculated with the use of cell-weighted averaging. Therefore, let F_b denote the fractions of a grid cell that are open for flow and F_s the fractions that are filled with liquid. This results in the following equations, as discussed in [9]:

$$\rho = \frac{F_s}{F_b}\rho_l + \frac{F_s - F_b}{F_b}\rho_g,$$
$$\mu = \frac{F_s}{F_b}\mu_l + \frac{F_s - F_b}{F_b}\mu_g.$$

In these equations, ρ_l and μ_l denote the incompressible liquid density and dynamic viscosity, respectively, and ρ_g and μ_g denote the compressible gas density and dynamic viscosity, respectively. The gas density is calculated using the adiabatic equation of state (4.1).

4.1.2 Numerical model

Depending on the kind of simulation, different input needs to be provided to ComFLOW and the pre-processors GEODEF and LIQDEF. The geometry definition of objects in the domain of simulation has to be described in the input file `geometry.in` and the initial fluid configuration should be described in `liquid.in`. Furthermore, the input file `comflow.in` contains all information about the size of the domain, the computational grid, the numerics and post-processing needed to run ComFLOW [9]. Note that the dimensions of the grid are given by `imax`, `jmax` and `kmax`. After running the pre-processors GEODEF and LIQDEF, the ComFLOW simmulation can be started. GEODEF has to be run for the definition of the geometry and LIQDEF for the initial fluid configuration. As discussed in [35], during a ComFLOW simulation, at every time step, grid cells are given labels to distinguish between fluid, air and boundary. The interior cells containing no fluid ($F_b > 0$ and $F_s = 0$) are labelled as E, empty cells. Non-empty cells ($F_s > 0$) adjacent to empty cells are labelled as S, surface cells. All the remaining cells are labelled as F, full cells. Cells which satisfy $F_s = F_b = 0$

and are adjacent to an interior cell are labelled as B, boundary cells. Otherwise, they are labelled as X, exterior cells [35]. An example of this label configuration is shown in Figure 4.1.

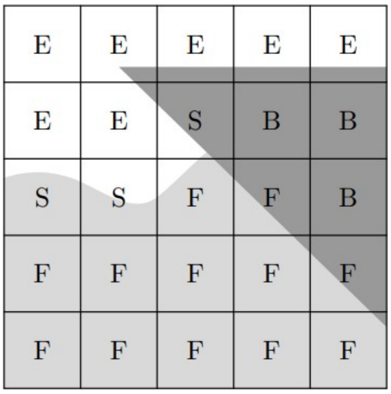


Figure 4.1: Two dimensional grid-cell labelling for an arbitrary geometry and liquid configuration. Dark, light shading and white represent solid body, liquid and air, respectively [9].

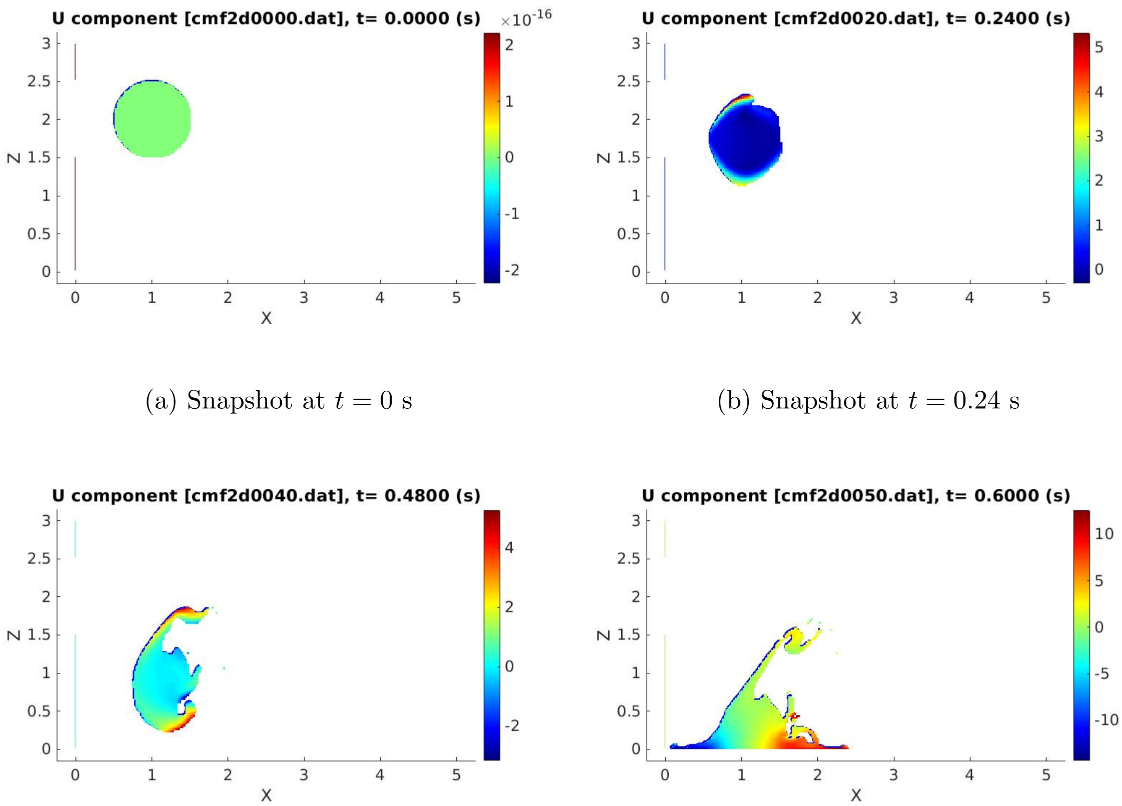
As discussed in [9], after the grid-cell labelling, the Navier-Stokes equations can be solved with the use of discretization in time and space. For the time discretisation, the first order accurate Forward Euler method or the second-order accurate Adams-Bashforth method can be used. The spatial discretization is based on the finite volume method. A choice can be made between (second-order) central discretisation and first or second order upwind discretisation. In this research, the Forward Euler method and upwind discretization are used. For the solution of the discretised Navier-Stokes equations, a Poisson equation for the pressure must be solved at each time step. For most two-phase flow simulations it is advantageous to use the MILU (Matrix Incomplete LU decomposition) or BiCGSTAB pressure solver. In this research, the BiCGSTAB + ILU(0), a preconditioner with special drop tolerance is used. When the pressure solution is found, the new velocity field is computed. Subsequently, the free surface is displaced using the Volume-of-Fluid (VOF) method combined with a local height function. Finally, the time step is adjusted using the CFL-number, $\eta = u\triangle t/\triangle x$ [35]. If the computed CFL-number is greater than `cflmax`, which is defined in the input file, the time step will be decreased. If the computed CFL-number is smaller than `cflmin` during 10 successive time steps, the time step will be doubled. The stability of these simulations depend on the CFL number η and the diffusion number $d = 2\mu\triangle t/(\triangle x)^2$, both have to be less than 1 [35].

4.2 ComFLOW simulations

The desired simulation is the two-phase simulation of a water droplet that moves from a person's mouth or nose to the ground. The water droplet should stay almost intact and not spray out over the whole domain. Furthermore, ideally the droplet has to move out of the mouth or nose with a velocity of approximately 50 m/s. To obtain the desired simulation several attempts have been made during this research. These attempts can be found below with an explanation of the input data and an evaluation of the output. The main input files that are used during these attempts can be found in Appendix B.

4.2.1 First attempt: air pushing against a sphere of water

The initial plan was to start with a rough 2-dimensional two-phase flow simulation of the water droplet. Firstly, it is assumed to have a very large droplet with a diameter of 1 meter, which starts at a height of 2 meters. Furthermore, an inflow boundary is added, with a wind current of 10 m/s between a height of 2.5 and 3.5 meters. This inflow boundary is implemented to cause a horizontal starting velocity of the droplet similar to the velocity v_{start} in Chapter 3. In order to run a 2-D simulation in the (XZ)-plane `jmax` has to be set equal to 1. During the simulation of the water droplet, several snapshots are made. Four snapshots can be found in Figure 4.2. Moreover, some relevant data can be found in Table 4.1. Note that this simulation has been run on a "standard" laptop computer.



(a) Snapshot at $t = 0$ s

(b) Snapshot at $t = 0.24$ s

(c) Snapshot at $t = 0.48$ s

(d) Snapshot at $t = 0.6$ s

Figure 4.2: Results of the first attempt using ComFLOW: moving air pushing against a sphere of water.

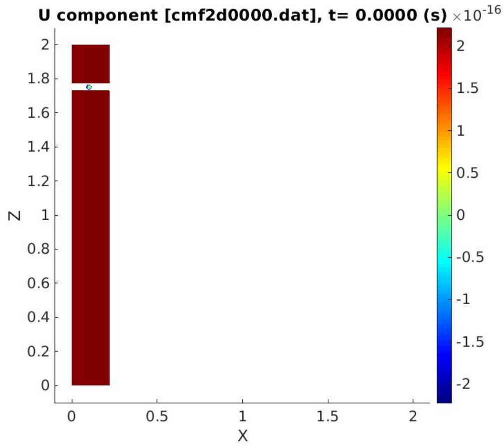
Quantity	**Given Value**
size of the droplet	circle with $r = 0.5$ m
density of the water	$1.0 \cdot 10^3$ kg/m^3
density of the air	1.0 kg/m^3
viscosity of the water	$1.0 \cdot 10^{-3}$ N·s/m^2
viscosity of the air	$1.71 \cdot 10^{-5}$ N·s/m^2
imax × kmax	200 × 120
cfl range	[0.2,0.5]
computational time	6 m

Table 4.1: Relevant data regarding the snapshots in Figure 4.2.

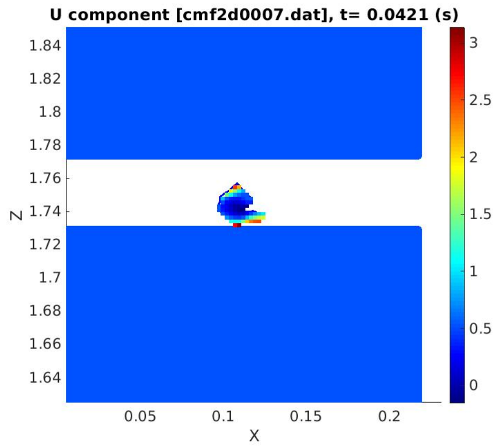
As shown in Figure 4.2a at $t = 0$, the composition of the figure looks like expected. There is a water droplet of a diameter 1 meter at a height of 2 meters and the lines at the left represent the inflow boundary of the wind current. However, when looking at the other three figures (4.2b,4.2c,4.2d), it can be seen that the droplet almost has no horizontal displacement. This is not in line with the desired output of the simulation. When looking at detailed information provided by the ComFLOW post-processor, it can be seen that the wind blows mainly around the droplet instead of against the droplet. As a results, the droplet only moves vertically. This can also be explained physically. Namely, the wind current will choose the route with the least resistance. Since the density of water is greater than the density of air, the wind will go around the droplet [30]. Despite the fact that the droplet only moves vertically, it can be seen that the water droplet deforms as a result of the forces acting on the droplet. Moreover, the droplet stays intact until it reaches the ground, where it splashes apart. The deformation and the fact that the droplet stays intact are actually positive points.

4.2.2 Second attempt: sphere in a channel

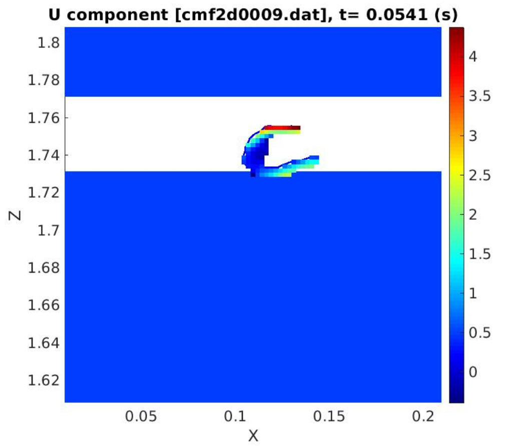
Using the findings from the previous section, a new attempt will be carried out for the 2-D simulation of the water droplet emerged from a person's mouth. A water droplet with a 2 cm diameter at a height of 1.75 meters is considered. Furthermore, a tube around the water droplet is implemented. The tube is implemented to ensure the wind current to mainly blow against the droplet instead of along. The wind current through the tube is 10 m/s and it is simulated with the use of an inflow boundary condition. During the simulation, several snapshots are made of which four can be found in Figure 4.3. Note that the last three figures are zoomed in to have a better view of the fluid dynamics. Moreover, some relevant data regarding the simulation can be found in Table 4.2. Note that this simulation and the following simulations in this chapter have been run on a remote system called Poseidon, which is more powerful than the laptop used for the previous simulation.



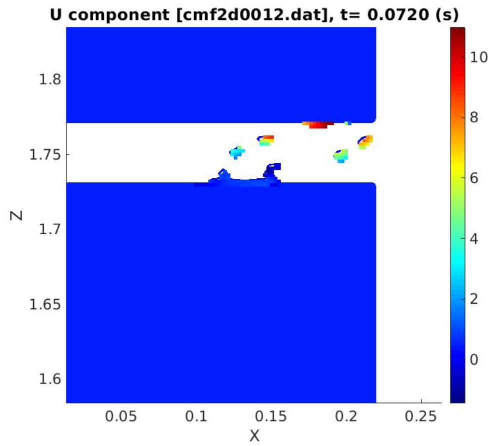
(a) Snapshot at $t = 0$ s



(b) Snapshot at $t = 0.0421$ s (zoomed in)



(c) Snapshot at $t = 0.0541$ s (zoomed in)



(d) Snapshot at $t = 0.072$ s (zoomed in)

Figure 4.3: Results of the second attempt: moving droplet as a result of air flow through a channel.

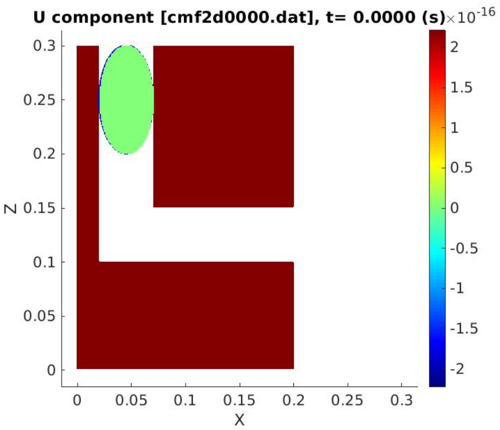
Quantity	**Given Value**
size of the droplet	circle with $r = 0.01$ m
density of the water	$1.0 \cdot 10^3$ kg/m^3
density of the air	1.0 kg/m^3
viscosity of the water	$1.0 \cdot 10^{-3}$ N·s/m^2
viscosity of the air	$1.71 \cdot 10^{-5}$ N·s/m^2
imax × kmax	500 × 500
cfl range	[0.2,0.5]
computational time	1 h 38 m

Table 4.2: Relevant data regarding the snapshots of Figure 4.3.

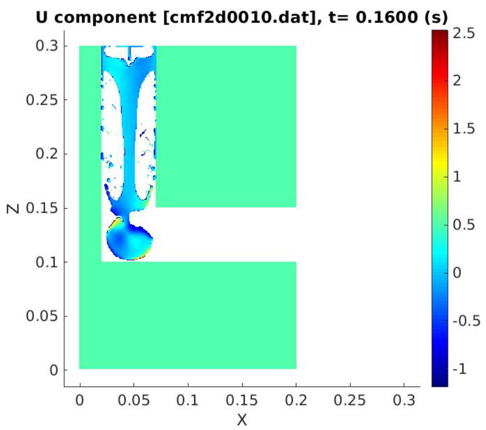
As can be seen in Figure 4.3, the snapshots show two rectangles that form the tube around the droplet. Figures 4.3b and 4.3c show that the wind current causes the droplet to move horizontally. However, in Figure 4.4d it can be seen that the droplet falls apart, which is not in line with the expected dynamics. The expected outcome was for the droplet to stay intact, at least largely. A possible cause of this can be the use of a too coarse grid, as can be seen from the small numbers of squares that are visible in the droplet. Moreover, the wind will again preferably choose the way around the droplet, which causes the droplet to spread into a string that eventually breaks out into smaller droplets. It must be noticed that the simulation takes roughly 20 times longer than the first attempt.

4.2.3 Third attempt: channel with an angle

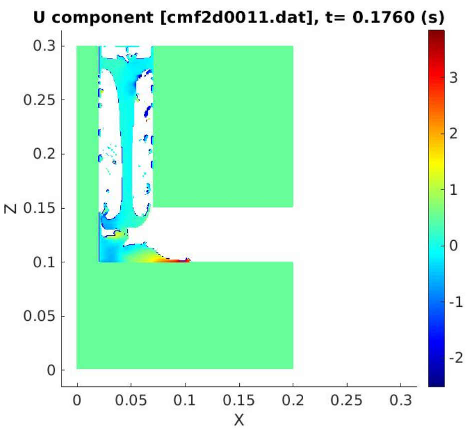
The first two attempts have shown that working with a wind current is probably not beneficial for the simulation. Therefore, gravity will be used to give the droplet a positive horizontal velocity. To be able to use gravity for a horizontal velocity, a set up such that the droplet will fall through a tube has to be introduced. For this attempt, a bigger droplet will be used to have a better insight in what happens. Next to that, a tube with an angle of 90 degrees will be made to obtain the final horizontal velocity. Four snapshots that are made during the simulation (Figure 4.4) as well as the table with relevant data can be found below (Table 4.3).



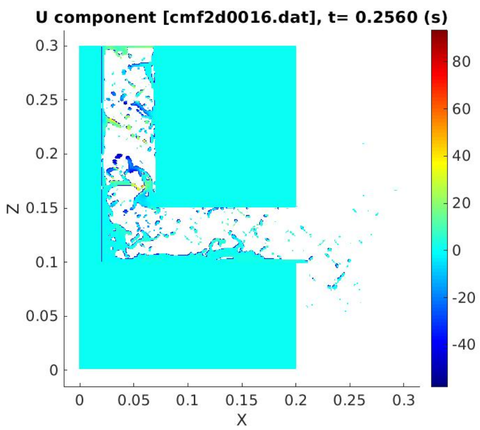
(a) Snapshot at $t = 0$ s



(b) Snapshot at $t = 0.16$ s



(c) Snapshot at $t = 0.176$ s



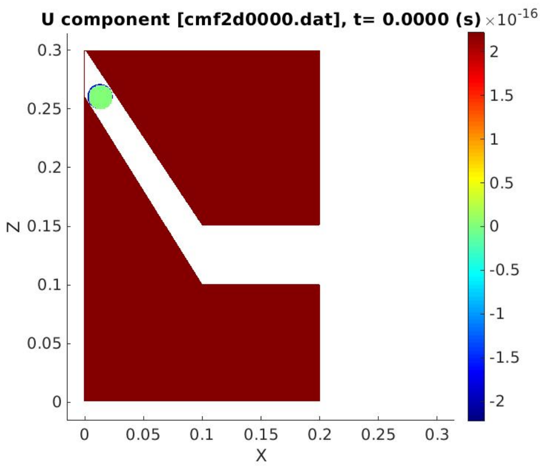
(d) Snapshot at $t = 0.256$ s

Figure 4.4: Results of the third attempt: moving droplet as a result of gravity due to a channel with a right angle.

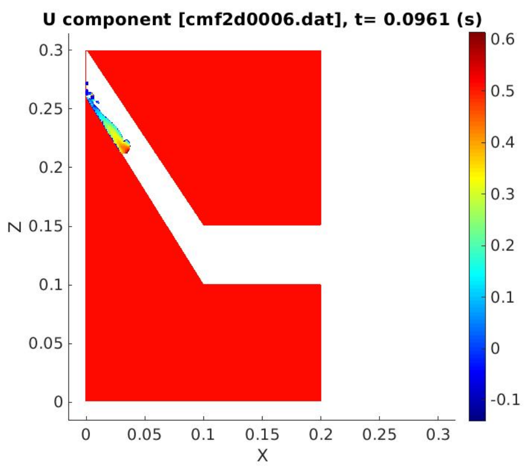
Quantity	**Given Value**
size of the droplet	circle with $r = 0.025$ m
density of the water	$1.0 \cdot 10^3$ kg/m^3
density of the air	1.0 kg/m^3
viscosity of the water	$1.0 \cdot 10^{-3}$ N·s/m^2
viscosity of the air	$1.71 \cdot 10^{-5}$ N·s/m^2
imax × kmax	300 × 300
cfl range	[0.2,0.5]
computational time	1 d 22 h 20 m

Table 4.3: Relevant data regarding the simulation in Figure 4.4.

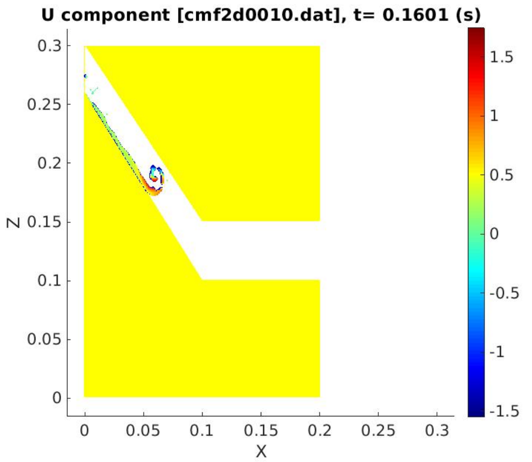
In Figure 4.4, it is shown that with the use of three rectangles a tube around the water droplet with a right angle is obtained. Furthermore, in Figure 4.4b it can be seen that the droplet falls and there is a droplet reaming at the bottom, yet already some water stays behind. The last two figures, 4.4c and 4.4d, show that the droplet fully splashes apart. However, the small water droplets that move out of the tube have a horizontal velocity, which is a positive result. It has to be noticed that the computational time is almost 2 days. It can be concluded that the use of gravity can be useful for the simulation. It is assumed that the right angle has a negative influence on keeping the water droplet intact. Therefore, the same technique with gravity will be used. However, with a different tube and a bit smaller water droplet. Some snapshots of this attempt (Figure 4.5) and the relevant data (Table 4.4) can be found below.



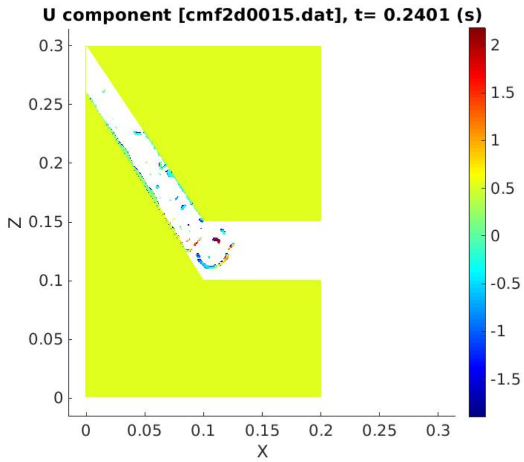
(a) Snapshot at $t = 0$ s



(b) Snapshot at $t = 0.0421$ s



(c) Snapshot at $t = 0.0541$ s



(d) Snapshot at $t = 0.072$ s

Figure 4.5: Results of the fourth attempt: moving droplet as a result of gravity due to a channel with an obtuse angle.

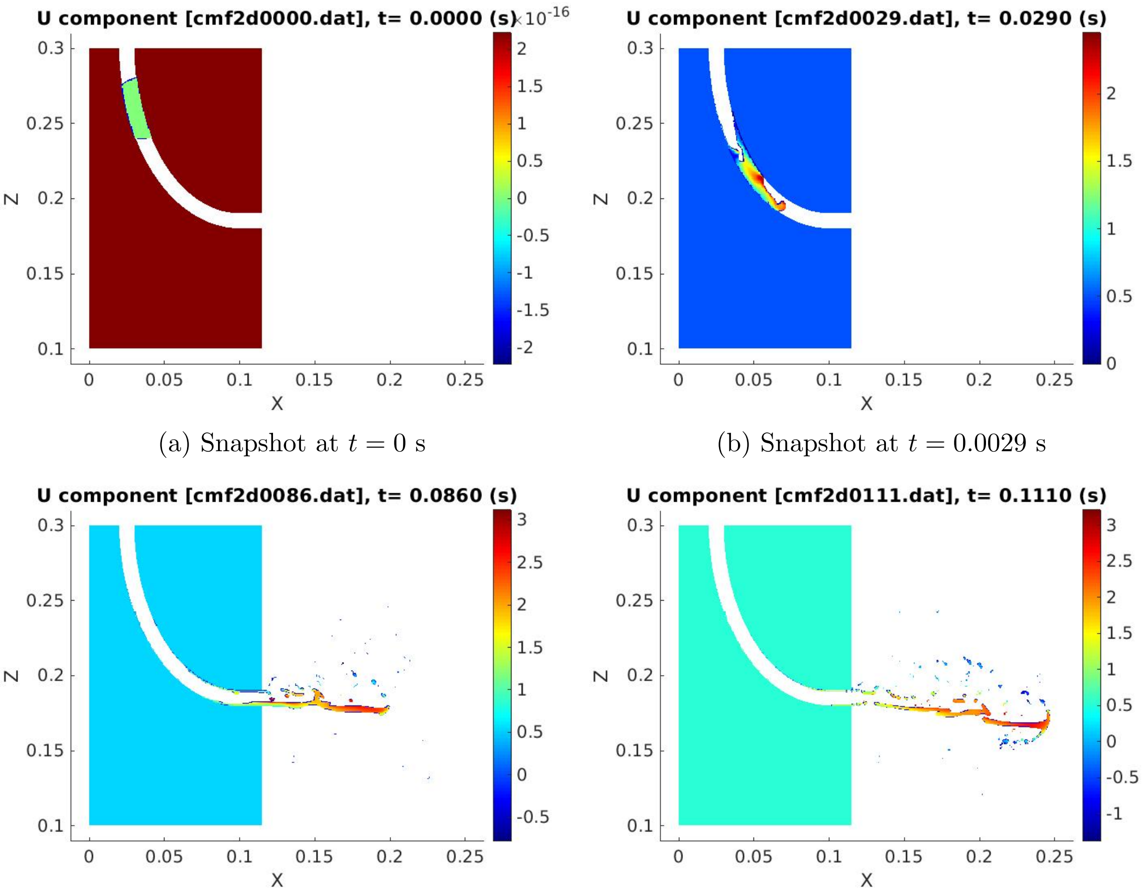
Quantity	**Given Value**
size of the droplet	circle with $r = 0.001$ m
density of the water	$1.0 \cdot 10^3$ kg/m^3
density of the air	1.0 kg/m^3
viscosity of the water	$1.0 \cdot 10^{-3}$ N·s/m^2
viscosity of the air	$1.71 \cdot 10^{-5}$ N·s/m^2
imax × kmax	300 × 300
cfl range	[0.2,0.5]
computational time	2 h 33 m

Table 4.4: Relevant data regarding the simulation in Figure 4.5.

As can be seen in Figure 4.5a, a new kind of tube with an obtuse angle is made using rectangles and a triangle. This causes the droplet to stay better intact at first, which can be seen in figures 4.5b and 4.5c. However, in Figure 4.5d the droplet again splashes apart. It is assumed that this is again caused by the sharp corner of the tube and again air goes around the droplet. Furthermore, it can be noted that the computational time is much shorter in comparison to the computational time of the previous simulation. This is due to the CFL limit $\eta = u\triangle t/\triangle x < 1$. In Figure 4.4 there are a lot of very small droplets with a high velocity. Therefore, $\triangle t$ has to decrease to compensate the high values of u in order to maintain stability. This causes a much longer computational time.

4.2.4 Final attempts: curved channel

In the attempts discussed in Section 4.2.3, it was noted that the set up to facilitate the use of gravity was slightly useful. However, the sharpness of the angles in the tubes caused the droplet to fall apart. Therefore, the set up is adjusted into a bending tube constructed with the use of ellipses and rectangles. To prevent the tube from vacuuming and accelerate the simulation, an inflow boundary with a velocity 2 m/s is used at the top. To test this attempt, a smaller domain and a bigger water droplet is chosen. The result can be found in Figure 4.6 and the relevant data in Table 4.5.



(a) Snapshot at $t = 0$ s

(b) Snapshot at $t = 0.0029$ s

(c) Snapshot at $t = 0.086$ s

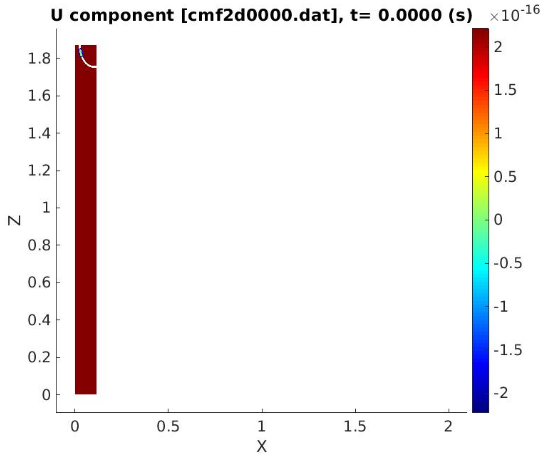
(d) Snapshot at $t = 0.111$ s

Figure 4.6: Results of the fifth attempt: moving droplet as a result of gravity due to a curved channel on a small domain.

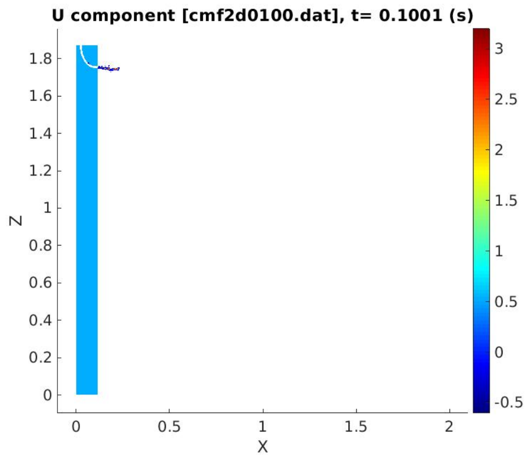
Quantity	**Given Value**
size of the droplet	circle with $r = 0.02$ m
density of the water	$1.0 \cdot 10^3$ kg/m^3
density of the air	1.0 kg/m^3
viscosity of the water	$1.0 \cdot 10^{-3}$ N·s/m^2
viscosity of the air	$1.71 \cdot 10^{-5}$ N·s/m^2
imax × kmax	375 × 300
cfl range	[0.2,0.6]

Table 4.5: Relevant data regarding the simulation in Figure 4.6.

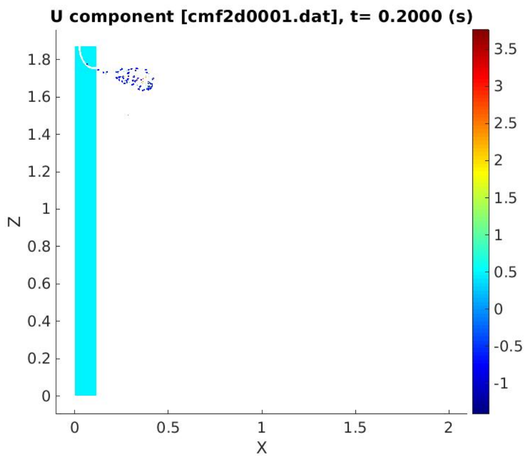
In Figure 4.6a, the position of the larger water droplet at the beginning of the simulation is shown. Figure 4.6b shows that the droplet "rolls" through the tube and stays intact. This is a large improvement over the previous attempt in Section 4.2.3. At the final stage (Figure 4.5c,4.5d), in which the droplet moves out of the tube, the droplet does not completely stay intact. However, it does move horizontally in a almost compact strip, which is positive. Therefore, the simulation will be enlarged to a realistic full scale domain. The results of this simulation can be found in Figure 4.7 and in Table 4.6 the relevant data is stated.



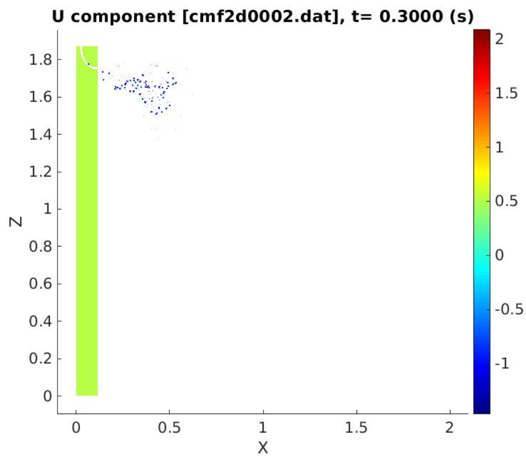
(a) Snapshot at $t = 0$ s



(b) Snapshot at $t = 0.1001$ s



(c) Snapshot at $t = 0.2$ s



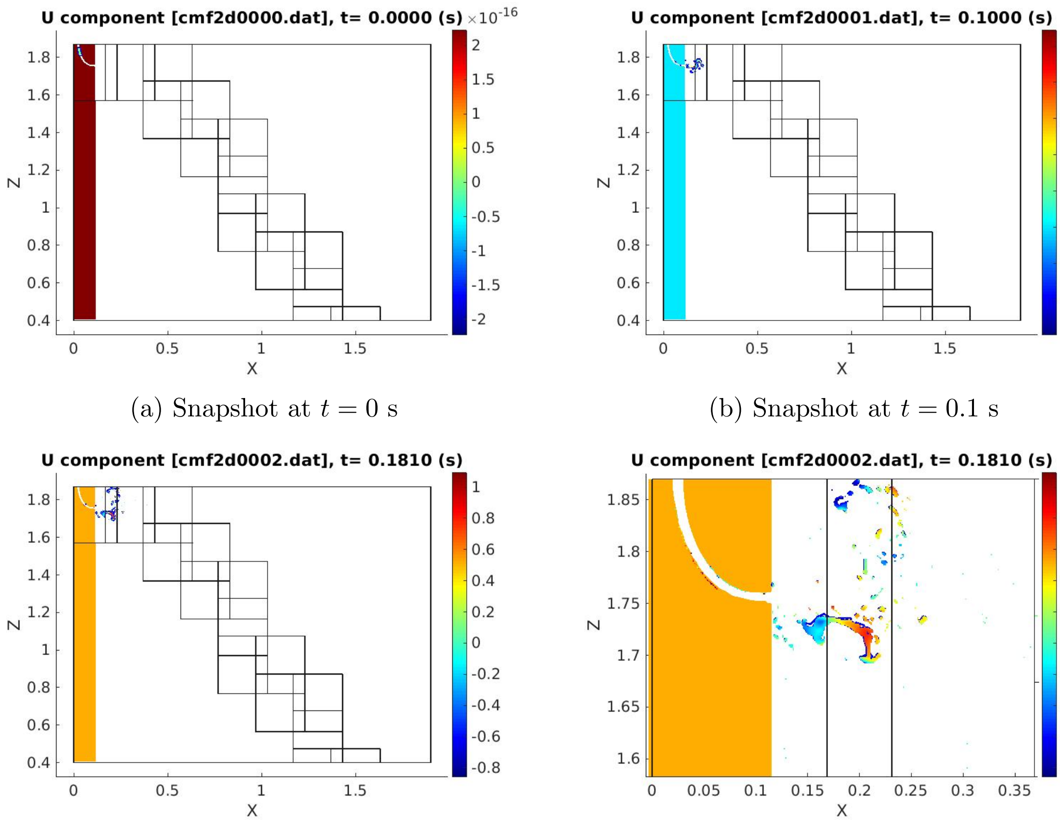
(d) Snapshot at $t = 0.3$ s

Figure 4.7: Results of the sixth attempt: moving droplet as a result of gravity due to a curved channel on a realistic full scale domain.

Quantity	**Given Value**
size of the droplet	circle with $r = 0.02$ m
density of the water	$1.0 \cdot 10^3$ kg/m^3
density of the air	1.0 kg/m^3
viscosity of the water	$1.0 \cdot 10^{-3}$ N·s/m^2
viscosity of the air	$1.71 \cdot 10^{-5}$ N·s/m^2
imax × kmax	2000 × 2000
cfl range	[0.2,0.6]
computational time	12 d 21 h 15 m

Table 4.6: Relevant data regarding the simulation in Figure 4.7.

In Figure 4.7a and 4.7b, the droplet moves out of the tube and takes the same strip form as in figures 4.6c and 4.6d. In Figure 4.7c, it can be seen that the spray is following a curve similar to the one discussed in Chapter 3 (Figure 3.2). Thus, the first three snapshots are rather satisfactory. However, as can been seen in Figure 4.7d, the droplet is transformed into a thinner spray. Besides, this simulation has taken circa 13 days to complete. Therefore, it is not a successful simulation. A possible cause of this failure can be that the grid is not fine enough. However, enlarging the grid means an even longer computational time. Therefore, local grid refinement is implemented. This is a method in which you can implement regions that have a finer grid, whereas the rest of the grid will have a coarse grid. This will speed up the simulation time and it will make the grid finer in the important regions. However, to be able to run this kind of simulation, the viscosity of the air apparently has to be enlarged for stability. This still gives a reliable result as it is of the same magnitude as artificial diffusion in case of $u = 2$ m/s. Artificial diffusion is caused by the use of an upwind discretization instead of a central discretization, which causes the diffusion coefficient effectively to increase with a factor $\frac{uh}{2}$ [36]. As in this chapter upwind discretization is used, it is allowed to increase the viscosity of the air. When using local grid refinement, an extra input file `grid.cfi` is needed in which the local grid and the refinement ratio are defined. The file for these definitions can be found in Appendix B.4.3. The local grids are defined with the use of the trajectory of the droplet found in Chapter 3. The result of this simulation is shown in Figure 4.8 and the relevant data can be found in Table 4.7.



(a) Snapshot at $t = 0$ s

(b) Snapshot at $t = 0.1$ s

(c) Snapshot at $t = 0.181$ s

(d) Zoomed in version of (c)

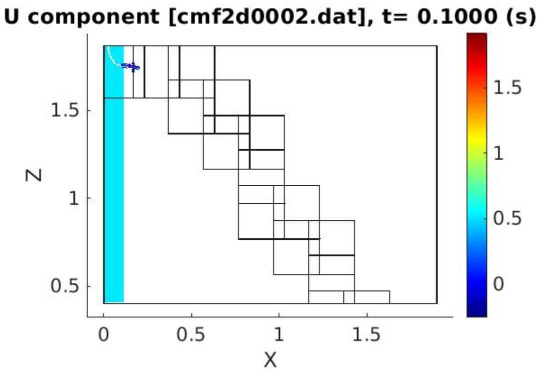
Figure 4.8: Results of the seventh attempt: moving droplet as a result of gravity due to a curved channel using local grid refinement.

Quantity	Given Value
size of the droplet	circle with $r = 0.02$ m
density of the water	$1.0 \cdot 10^3$ kg/m^3
density of the air	1.0 kg/m^3
viscosity of the water	$1.0 \cdot 10^{-3}$ N·s/m^2
viscosity of the air	$1.0 \cdot 10^{-3}$ N·s/m^2
imax × kmax	304 × 240, refinement ratio = 5
cfl range	[0.2,0.5]
computational time	1 d 21 h 56 m

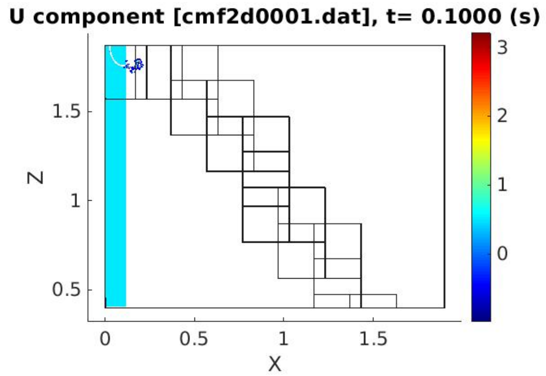
Table 4.7: relevant data regarding the simulation in Figure 4.8.

The grid refinement blocks are shown in Figure 4.8. They have a small overlap to prevent gaps between the blocks. Moreover, from Figures 4.8b and 4.8c it could be concluded that the droplets fall apart and move upwards. This is even more clear in the zoomed Figure 4.8d. The fact that the spray moves upwards to the ceiling is unrealistic. A cause of this failed simulation can be that the grid is still not fine enough and that ComFLOW sees the overlap of the blocks as an artificial edge. Moreover, an explanation of the upward spray can be that there is not enough water present in some grid cells at each time step. ComFLOW calculates the amount of water that has to be moved to the adjacent cell. However, if there is not much water present in a cell ComFLOW does not exactly now where it is located. Consequently, it has complications in which direction the small amount of water goes, which can result in a spray moving upwards.

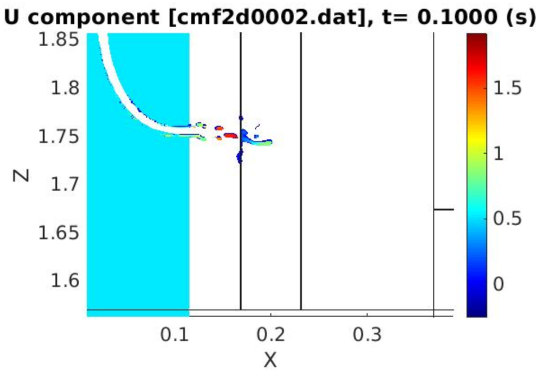
In this research, a water droplet is used in the simulation as it is quite similar to a mucus droplet. Namely, a mucus droplet exists for 98 percent of water [8]. However, a mucus droplet is a bit more viscous than water. Therefore, the same simulation as above is taken in which the viscosity of the water is enlarged with a factor 10. In Figure 4.9 a comparison between these simulations at $t = 1$ s can be seen. In Table 4.8 the relevant data of the simulation with a larger water viscosity is shown.



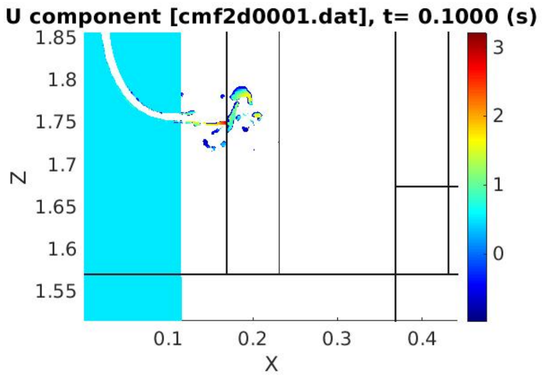
(a) Snapshot at $t = 0.1$ s, with a larger viscosity of the water



(b) Snapshot at $t = 0.1$ s, with the standard water viscosity



(c) Zoomed in version of (a)



(d) Zoomed in version of (b)

Figure 4.9: Results of the seventh attempt: with two different viscosity values of mucus-like water, each at $t = 0.1$ s.

Quantity	**Given Value**
size of the droplet	circle with $r = 0.02$ m
density of the water	$1.0 \cdot 10^3$ kg/m^3
density of the air	1.0 kg/m^3
viscosity of the water	$1.0 \cdot 10^{-2}$ N·s/m^2
viscosity of the air	$1.0 \cdot 10^{-3}$ N·s/m^2
imax $\times$ kmax	304×240, refinement ratio $= 5$
cfl range	[0.2,0.5]
computational time	6 d 9 h 6 m

Table 4.8: Relevant data regarding the simulation in Figure 4.9.

In Figure 4.9 it is shown that enlarging the viscosity has a positive effect for the simulation of a flying droplet. In Figure 4.9c, a water strip is observed that is almost compact and moves downwards. On the other hand, in Figure 4.9d the water strip falls a bit more apart and moves upward. Hence, the use of a bigger viscosity causes the droplet to longer stay together and causes a more realistic trajectory of the droplet. However, when comparing the required computational times, the use of a higher viscosity is very computationally expensive. This can be explained with the use of the diffusion number (see Section 4.1.2), when the viscosity increases the time step has to decrease for the simulation to remain stable. Moreover, looking at Figure 4.10, at $t = 0.222$ s the droplet will eventually spray out and a part of the water moves vertically to the ground. Hence, on the one hand increasing the viscosity causes the droplet to stay longer together, yet on the other hand it gives a far larger computational time.

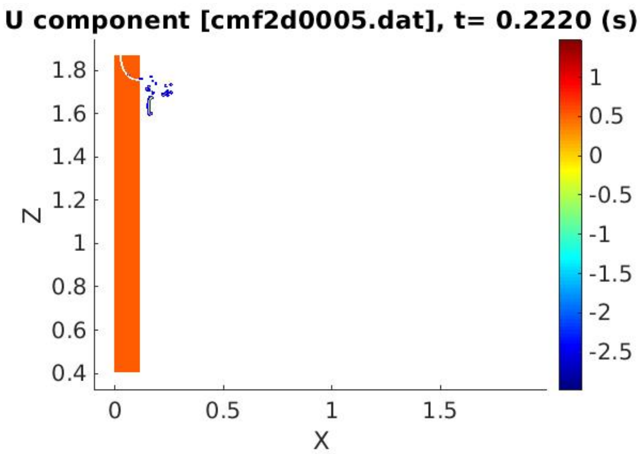
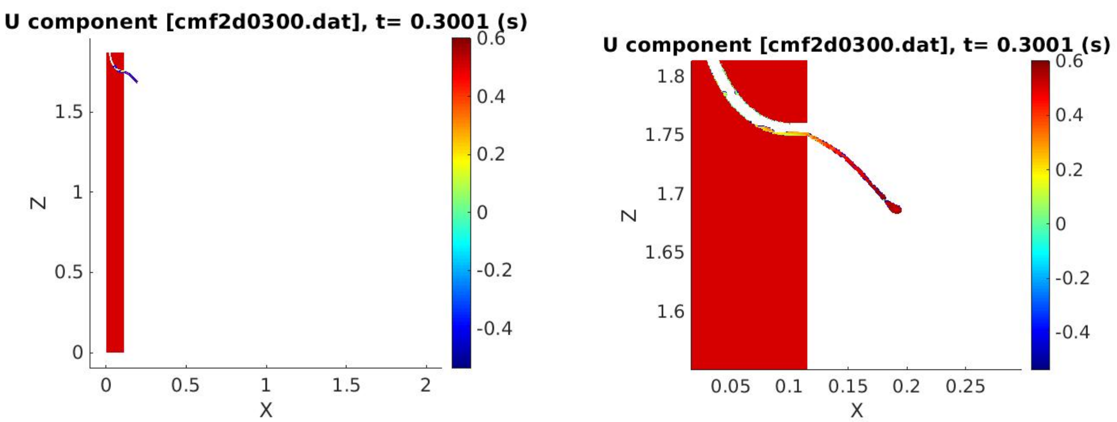


Figure 4.10: Results of the seventh attempt: using a higher viscosity causes the droplet to stay together much longer.

To conclude, in this section only failed simulations can be found since the droplet sprays out too much. It is assumed that this is mainly caused by the too coarse grid, although using very fine grids did not give much improvement. However, it is seen that the use of a higher viscosity causes the droplet to stay longer together. It is also studied if increasing the contact angle has a positive effect on the simulation. Unfortunately, this is not the case. Next to varying the contact angle also the use of a one-phase simulation is investigated. In Figure 4.11, the same set up can be seen as in Figure 4.7. However, in this simulation a one-phase model is used instead of a two-phase simulation. It is shown that the droplet stays intact up to $t = 3$ s, which is the longest time seen so far. It can be concluded that ComFLOW "struggles" with a two-phase approach. However, for a realistic trajectory it was found in Chapter 3 that a two-phase simulation is really needed. Hence, it can be concluded that ComFLOW does not give the preferred trajectory of a water droplet.



(a) Result

(b) Zoomed in version of a

Figure 4.11: Results of a one-phase ComFLOW simulation.

Chapter 5

Conclusion

This study aimed to investigate the social distance measure from a mathematical perspective. In order to achieve this, a 2-dimensional model was set up in ComFLOW to simulate the trajectory of a water droplet from a person's mouth or nose to the ground. By analysing several attempts from ComFLOW, this study also shows whether ComFLOW is the appropriate program for simulating a flying droplet.

After reviewing the literature on COVID-19 and the dynamics of sneezing and coughing, an ODE model to verify the simulations from ComFLOW was obtained. This model proved that a two-phase approach is needed in the simulation of a flying water droplet, since air resistance has a large effect on the trajectory. Furthermore, it was shown that at the beginning of the simulation the velocity of the water droplet did not have a large influence on the horizontal motion.

In the final attempts of the simulations with ComFLOW, the initial position of the droplet is located in a smooth tube made of ellipses and rectangles. This set up is used to give the droplet a positive horizontal velocity with the use of gravity. The simulations have shown that a credible simulation of a water droplet is very computationally expensive in ComFLOW. All the attempts caused the droplet to spray out too much, mostly due to the coarseness of the grid. Increasing the viscosity of the water is to some extent beneficial for the results, yet it causes a longer computational time. In conclusion, ComFLOW is a not an ideal program for the simulation of a flying water droplet in air. Therefore, unfortunately nothing can be said about which countries have chosen the "best" social restriction measures.

To obtain better results of the ComFLOW simulations, future studies could use a more powerful computer which can handle super fine grids. Otherwise, another program should be chosen or developed for the simulation of a flying water droplet.

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Appendix A

MATLAB files

A.1 Function files

ODE_ax.m

```
%INPUT
%v_x              the velocity of the droplet decomposed in the ...
    x-direction
%A                the area of the droplet
%Cd               the drag coefficient
%m                the mass of the droplet
%rho              the density of the air
%v_mag            the magnitude of the velocity

%OUTPUT
%f                the decomposition of the acceleration of the droplet
%                 in the x-derection

function f=ODE_ax(v_x,A,Cd,m,rho,v_mag)
k = 1/2*rho*Cd*A*(v_x)^2;
f= -k/m*v_x*v_mag;
end
```

ODE_ay.m

```
%INPUT
%v_y              the velocity of the droplet decomposed in the ...
    y-direction
%A                the area of the droplet
%Cd               the drag coefficient
%g                the gravity force constant
%m                the mass of the droplet
%rho              the density of the air
%v_mag            the magnitude of the velocity

%OUTPUT
%f                the decomposition of the acceleration of the droplet
%                 in the y-derection

function f=ODE_ay(v_y,A,Cd,g,m,rho,v_mag)
k = 1/2*rho*Cd*A*(v_y)^2;
f= -g-k/m*v_y*v_mag;
end
```

magnitude.m

```
%INPUT
%v_x        the velocity of the droplet decomposed in the x-direction
%v_y        the velocity of the droplet decomposed in the y-direction

%OUTPUT
%v_mag      the magnitude of the velocity vector v

function v_mag=magnitude(v_x,v_y)
v_mag=sqrt((v_x)^2+(v_y)^2);
end
```

motion_without_air_resistance.m

```
%INPUT
%x          x-position of the droplet without air resistance
%h          height from which the droplet starts with falling
%g          the gravity force constant
%v_start    starting velocity of the droplet

%OUTPUT
%y          y-position at x of the droplet without air resistance

function y=motion_without_air_resistance(x,h,g,v_start)
y=h-g/(2*(v_start)^2)*x.^2;
end
```

A.2 Running files

A.2.1 Motion of droplet with air resistance

motion_of_droplet.m

```
%DEFINING PARAMETERS
A=1E-6; %area of the droplet (m^2)
V=1E-9; %volume of the droplet (m^3)
rho_d=997; %density of the droplet (kg/m^3)
Cd=0.47; %drag coeffienct
g=9.81; %gravity force constant (m/s^2)
m=rho_d*V; %mass of the droplet (kg)
rho=1.2041; %density of the air (kg/m^3)
H=1.75; %height of the mouth (m)
v_start=50; %starting velocity (m/s)

%INITIAL CONDITIONS
x(1)=0;
y(1)=H;
v_x(1)=v_start;
v_y(1)=0;

%SETTINGS
h=0.00001; %stepsize
t=200000; %time

%solving the ODE with air resistance, with two times forward Euler
for n=1:t
```

```
    v_x(n+1) = v_x(n) + ...
        h*ODE_ax(v_x(n),A,Cd,m,rho,magnitude(v_x(n),v_y(n)));
    v_y(n+1) = v_y(n) + ...
        h*ODE_ay(v_y(n),A,Cd,g,m,rho,magnitude(v_x(n),v_y(n)));
    x(n+1) = x(n) + h*v_x(n);
    y(n+1) = y(n) + h*v_y(n);
    if y(n+1)≤0
        disp(x(n+1))
        break
    end
end

%plotting the results
plot(x,y)
hold on
line(xlim(), [0,0], 'LineWidth', 1, 'Color', 'k');
title('Motion of the droplet')
xlabel('distance (m)')
ylabel('height (m)')
```

A.2.2 Motion of the droplet with and without air resistance

motion_droplet_with_and_without_air.m

```
%DEFINING PARAMETERS
A=1E-6; %area of the droplet (m^2)
V=1E-9; %volume of the droplet (m^3)
rho_d=997; %density of the droplet (kg/m^3)
Cd=0.47; %drag coeffient
g=9.81; %gravity force constant (m/s^2)
m=rho_d*V; %mass of the droplet (kg)
rho=1.2041; %density of the air (kg/m^3)
H=1.75; %height of the mouth (m)
v_start=50; %starting velocity (m/s)

%INITIAL CONDITIONS
x(1)=0;
y(1)=H;
v_x(1)=v_start;
v_y(1)=0;

%settings
h=0.00001; %stepsize
t=20000000; %time

%solving the ODE with air resistance, with two times forward Euler
for n=1:t
    v_x(n+1) = v_x(n) + ...
        h*ODE_ax(v_x(n),A,Cd,m,rho,magnitude(v_x(n),v_y(n)));
    v_y(n+1) = v_y(n) + ...
        h*ODE_ay(v_y(n),A,Cd,g,m,rho,magnitude(v_x(n),v_y(n)));
    x(n+1) = x(n) + h*v_x(n);
    y(n+1) = y(n) + h*v_y(n);
    if y(n+1)≤0
        disp(x(n+1))
        break
    end
```

```
end

%motion of the droplet without air resistance
for i=1:t
    x2(i)=h*(i-1);
    y2(i)=motion_without_air_resistance(x2(i),H,g,v_start);
    if y2(i)≤0
        disp(x2(i))
        break
    end
end

%plotting the results
plot(x,y)
hold on
plot(x2,y2)
line(xlim(), [0,0], 'LineWidth', 1, 'Color', 'k');
title('Motion of the droplet')
xlabel('distance (m)')
ylabel('height (m)')
legend('with air resistance','without air resistance')
```

A.2.3 Motion of the droplet with air resistance and different velocities

motion_droplet_different_v.m

```
%DEFINING PARAMETERS
A=1E-6; %area of the droplet (m^2)
V=1E-9; %volume of the droplet (m^3)
rho_d=997; %density of the droplet (kg/m^3)
Cd=0.47; %drag coeffiecnt
g=9.81;%gravity force constant (m/s^2)
m=rho_d*V; %mass of the droplet (kg)
rho=1.2041; %density of the air (kg/m^3)
H=1.75; %height of the mouth (m)
v_start=50; %starting velocity (m/s)

%INITIAL CONDITIONS
x(1)=0;
y(1)=H;

v_y(1)=0;

%SETTINGS
h=0.00001; %stepsize
t=2000000; %time

%solving the ODE with air resistance, with two times forward Euler
for j=1:3
    v_x(1)=10 + 20*(j-1);
for n=1:t
    v_x(n+1) = v_x(n) + ...
        h*ODE_ax(v_x(n),A,Cd,m,rho,magnitude(v_x(n),v_y(n)));
    v_y(n+1) = v_y(n) + ...
        h*ODE_ay(v_y(n),A,Cd,g,m,rho,magnitude(v_x(n),v_y(n)));
    x(n+1) = x(n) + h*v_x(n);
```

```
    y(n+1) = y(n) + h*v_y(n);
    if y(n+1)<=0
        disp(x(n+1))
        break
    end
end
plot(x,y)
hold on
end

%plotting the results
line(xlim(), [0,0], 'LineWidth', 1, 'Color', 'k');
title('Motion of the droplet')
xlabel('distance (m)')
ylabel('height (m)')
legend('v=10 m/s','v=30 m/s','v=50 m/s')
```

Appendix B

ComFLOW files

B.1 First attempt

comflow.in

```
--@v312-------------------------------------------------------------------
-- Title -----------------------------------------------------------------
2D moving droplet
--------------------------------------------------------------------------
slosh   mvbd     twph   nproc
1       0        1      1
--------------------------------------------------------------------------
-- domain definition -----------------------------------------------------
xmin    xmax    ymin    ymax    zmin zmax
0 5.0 -1 1 0.0 3.0
--------------------------------------------------------------------------
-- green water parameters ------------------------------------------------
grnwtr
0
--------------------------------------------------------------------------
high    low     length
0.0     0.0     0.0
--------------------------------------------------------------------------
width   a       b
0.0     0.0     0.0
--------------------------------------------------------------------------
-- definition initial liquid configuration -------------------------------
liqcnf lqxmin  lqxmax  lqymin  lqymax  lqzmin  lqzmax
0      -8.0    8.0     -8.0    8.0     -10.0   7.0
--------------------------------------------------------------------------
-- definition of incoming wave -------------------------------------------
wave  wvstart  period   wheight  xcrest  waterd  ramp*  order  curr beta
0     0        0  0        0       0       0      0      0.0  0.0
ramp  val1  val2
0     0.0   0.0
--------------------------------------------------------------------------
-- definition of in- and outflow boundaries ------------------------------
```

```
nrio
2
i/o     plane   xmin    xmax    ymin    ymax    zmin    zmax    iospec
iostart iofull
101  1       0.      0. -1.      1. 1.5 2.5     10.     0.     0.1
2       1       5.      5. -1.      1. 0. 3.
------------------------------------------------------------------------
-- partial slip --------------------------------------------------------
pscnf psl
0 0.0
------------------------------------------------------------------------
-- absorbing boundary condition ----------------------------------------
bcl bcr     a0 a1 b1    kh
1 1 1.05 0.14 0.32  1.0
------------------------------------------------------------------------
-- definition of numerical beach in positive x-direction ---------------
numbch  dampto* slope   bxstart
0       0       0.05    134
------------------------------------------------------------------------
-- physical parameters -------------------------------------------------
rho1    rho2    mu1     mu2     sigma   theta  patm   gamma
1.0e3   1.0     1.0e-3  1.71e-5 73.0E-6     90.0   1.0e5  1.4
------------------------------------------------------------------------
-- grid parameters -----------------------------------------------------
griddef
1
imax    jmax    kmax    xc      yc      zc      sx      sy      sz
200     1       120     0.0     0.0     0.0     1.0     1.0     1.0
------------------------------------------------------------------------
-- numerical parameters ------------------------------------------------
eps     omega   itmax   alpha   feab0  feab1  feab2   nrintp  fslinext
1.0E-6  1.0     1000    1.0     0.0    1.0    0.0     4       1
------------------------------------------------------------------------
-- numerical parameters two-phase flow ---------------------------------
solver extrap  restol  imptol  upwind  imprel  irhoav  itscr droptol droptol2
5      0       1.0E-8  1.0E-3  1       1.0     1       0  5E-3  1E-6
------------------------------------------------------------------------
-- time parameters/cfl number ------------------------------------------
dt      tmax    dtmax   cfl     cflmin  cflmax  divl
0.01    0.6     0.1     1       0.2     0.5     0
------------------------------------------------------------------------
-- free surface methods ------------------------------------------------
vofmth   vofcor  divl
1         2       0
------------------------------------------------------------------------
-- gravitation ---------------------------------------------------------
gravx   gravy   gravz   ginrt   finrt
0.0     0.0     -9.81       0       0
```

```
-------------------------------------------------------------------------
-- motion of coordinate system ------------------------------------------
motionframe
0
amplx   freqx   amply   freqy   amplz   freqz
0.0     0.0     0.0     0.0     0.0     0.0
-------------------------------------------------------------------------
omex    omey    omez    x0      y0      z0
0.0     0.0     0.0     0.0     0.0     0.0
-------------------------------------------------------------------------
-- autosave -------------------------------------------------------------
load    nsave
0       0
-------------------------------------------------------------------------
-- post-processing: snapshots/screen print/center of mass --------------
npm2d   npm3d   compr   nprnt   ntcom
50      0       0       1000     0
-------------------------------------------------------------------------
npmslic nyz     nxz     nxy
0       0       0       0
planeyz
planexz
planexy
-------------------------------------------------------------------------
-- directory name for snapshots ----------------------------------------
pathname snapshot data:
data/
-------------------------------------------------------------------------
-- fill boxes, force boxes and flux boxes-------------------------------
nfillb  ntfill
0       2000
xl      xr      yl      yr      zl      zr
-------------------------------------------------------------------------
nfrcb   ntfrc
0      2000
xl      xr      yl      yr      zl      zr     mv meth
-------------------------------------------------------------------------
nfluxb  ntflux
0       0
xl      xr      yl      yr      zl      zr
-------------------------------------------------------------------------
nrelwh  ntrelwh
0       0
xl      xr      yl      yr      zl      zr
-------------------------------------------------------------------------
-- stream line/particle path --------------- ----------------------------
npartp  npartl  npartc  ntpart
0       0       0       0
```

```
xpt     ypt     zpt     tstrt                           <- points
xl      xr      yl      yr      zl      zr      tstrt   <- lines
xc      yc      zc      radius  orient  tstrt           <- circles
-------------------------------------------------------------------------
-- monitor points -------------------------------------------------------
nmntrp  nmntrl  nmntrc  ntmntr
0       0       0       1000
xpt     ypt     zpt     mvp                             <- points
xl      xr      yl      yr      zl      zr              <- lines
xc      yc      zc      radius  orient                  <- circles
-------------------------------------------------------------------------
-- special boxes --------------------------------------------------------
nrboxes tstart sbuvw
0       0.0    0
xmin    xmax    ymin    ymax    zmin    zmax
-------------------------------------------------------------------------
```

liquid.in

```
13 0 1
1 2
0.5 0.5
```

B.2 Second attempt

liquid.in

```
13 0 1
0.2 1.75
0.01 0.01
```

geometry.in

```
12 0 0
0 0
0.22 0
0.22 1.73
0 1.73
12 0 0
0 1.77
0.22 1.77
0.22 2
0 2
```

B.3 Third attempt

B.3.1 Right angle

liquid.in

```
13 0 1
```

```
0.045 0.25
0.025 0.05
```

geometry.in

```
12 0 0
0 0
0.2 0
0.2 0.1
0 0.1
12 0 0
0 0.1
0.02 0.1
0.02 0.3
0 0.3
12 0 0
0.07 0.15
0.2 0.15
0.2 0.3
0.07 0.3
```

B.3.2 Obtuse angle

liquid.in

```
13 0 1
0.013 0.26
0.01 0.01
```

geometry.in

```
12 0 0
0 0
0.2 0
0.2 0.1
0 0.1
11 0 0
0 0.1
0.1 0.1
0 0.26
12 0 0
0 0.3
0.2 0.3
0.2 0.15
0.1 0.15
```

B.4 Final attempt

B.4.1 General idea

liquid.in

```
13 0 1
0.035 0.26
0.02 0.02
```

geometry.in

```
12 0 0
0.00 0.00
0.15 0.00
0.15 0.30
0.00 0.30
13 1 0
0.10 0.30
0.08 0.12
13 0 0
0.10 0.30
0.07 0.11
12 1 0
0.10 0.00
0.25 0.00
0.25 0.30
0.10 0.30
12 0 0
0.10 0.00
0.115 0.00
0.115 0.18
0.10 0.18
12 0 0
0.10 0.19
0.115 0.19
0.115 0.30
0.10 0.30
```

B.4.2 Realistic domain

liquid.in

```
13 0 1
0.035 1.83
0.02 0.02
```

geometry.in

```
12 0 0
0.00 0.00
0.15 0.00
0.15 1.87
0.00 1.87
13 1 0
0.10 1.87
```

```
0.08 0.12
13 0 0
0.10 1.87
0.07 0.11
12 1 0
0.10 0.00
0.25 0.00
0.25 1.87
0.10 1.87
12 0 0
0.10 0.00
0.115 0.00
0.115 1.75
0.10 1.75
12 0 0
0.10 1.76
0.115 1.76
0.115 1.87
0.10 1.87
```

B.4.3 Grid refinement

`liquid.in`

```
13 0 1
0.035 1.83
0.02 0.02
```

`geometry.in`

```
12 0 0
0.00 0.00
0.15 0.00
0.15 1.87
0.00 1.87
13 1 0
0.10 1.87
0.08 0.12
13 0 0
0.10 1.87
0.07 0.11
12 1 0
0.10 0.00
0.25 0.00
0.25 1.87
0.10 1.87
12 0 0
0.10 0.00
0.115 0.00
```

```
0.115 1.75
0.10 1.75
12 0 0
0.10 1.76
0.115 1.76
0.115 1.87
0.10 1.87
```

grid.cfi


```
<?xml version="1.0" encoding="utf-8"?>
<comflow version="3.9">

<!--================================================
==== Grid
================================================-->
   <grid>
      <dimension>304 1 240</dimension>

      <!-- refinement ratios -->
      <refinement>5 5 5</refinement>

      <!-- coarse base grid -->
      <subgrid level="0" everywhere="1"/>

<subgrid level="1"> -0.03 0.23 0 0  1.57 1.88 </subgrid>
<subgrid level="1">  0.17 0.43 0 0  1.57 1.88 </subgrid>
<subgrid level="1">  0.37 0.63 0 0  1.57 1.88 </subgrid>
<subgrid level="1">  0.37 0.63 0 0  1.37 1.67 </subgrid>
<subgrid level="1">  0.57 0.83 0 0  1.37 1.67 </subgrid>
<subgrid level="1">  0.57 0.83 0 0  1.17 1.47 </subgrid>
<subgrid level="1">  0.77 1.03 0 0  1.17 1.47 </subgrid>
<subgrid level="1">  0.77 1.03 0 0  0.97 1.27 </subgrid>
<subgrid level="1">  0.77 1.03 0 0  0.77 1.07 </subgrid>
<subgrid level="1">  0.97 1.23 0 0  0.77 1.07 </subgrid>
<subgrid level="1">  0.97 1.23 0 0  0.57 0.87 </subgrid>
<subgrid level="1">  1.17 1.43 0 0  0.57 0.87 </subgrid>
<subgrid level="1">  1.17 1.43 0 0  0.37 0.67 </subgrid>
<subgrid level="1">  1.17 1.43 0 0  0.17 0.47 </subgrid>
<subgrid level="1">  1.37 1.63 0 0  0.17 0.47 </subgrid>
<subgrid level="1">  1.37 1.63 0 0 -0.03 0.27 </subgrid>

      </grid>

</comflow>
```