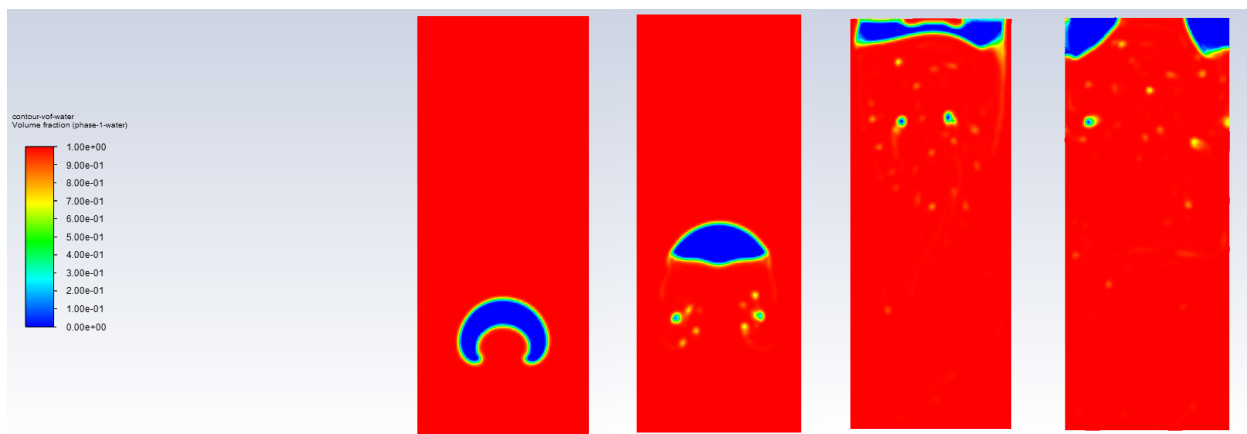


TECHNIQUES NUMERIQUES DE SEPARATION HUILE-EAU



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Cette page est laissée intentionnellement vierge.

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Objectifs du projet :

The main goal of this project is to get familiar with Computational Fluid Dynamics, which are often used by engineers in their daily work. It is mainly about solving equations in the domain of fluid flow using numerical tools. To approach this subject we went through a quick discovery of the theory of fluid mechanics and multiphase problems. We also studied the functioning of a few numerical methods, before moving on to practice by realizing several simulations using the Ansys Fluent software.

Mots-clefs du projet : **Fluid dynamics, CFD, Multiphase system, Ansys Fluent**

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1. INTRODUCTION

Fluid mechanics are a very complex field of physics, but also one of the most important and useful. The applications of it are countless, and can be found everywhere in our lives, from the cars we use to go to work, to the weather forecasts we watch to know whether, yes or no, we should take that raincoat. Therefore it is interesting for us, as humans, to try and understand parts of it. As for our interest as engineers, it is even bigger. Indeed fluid mechanics are a reunion of many fields of physics such as mechanics or thermodynamics, together with mathematical analysis. That is why, whether we intend to continue our study of physics or not, it is scientifically engaging to learn about it. The goal of this project is to provide an overview of this domain through some specific problems that we had to do a numerical simulation for. The objective for us was therefore threefold: to study the behaviour of multiphase systems, to discover the numerical methods to solve problems involving multiphase systems, and finally to learn how to use Ansys Fluent.

In this report, we presented first the project management during the semester, as it was a very important part, especially because of the actual context of not being able to see each other. Then we made a summary of the theoretical knowledge we acquired about fluid mechanics, to move on afterwards to the numerical techniques that we studied. Finally we exposed the different simulations that we actually did using Ansys Fluent.

2. METHODOLOGY/ORGANISATION AS A GROUP

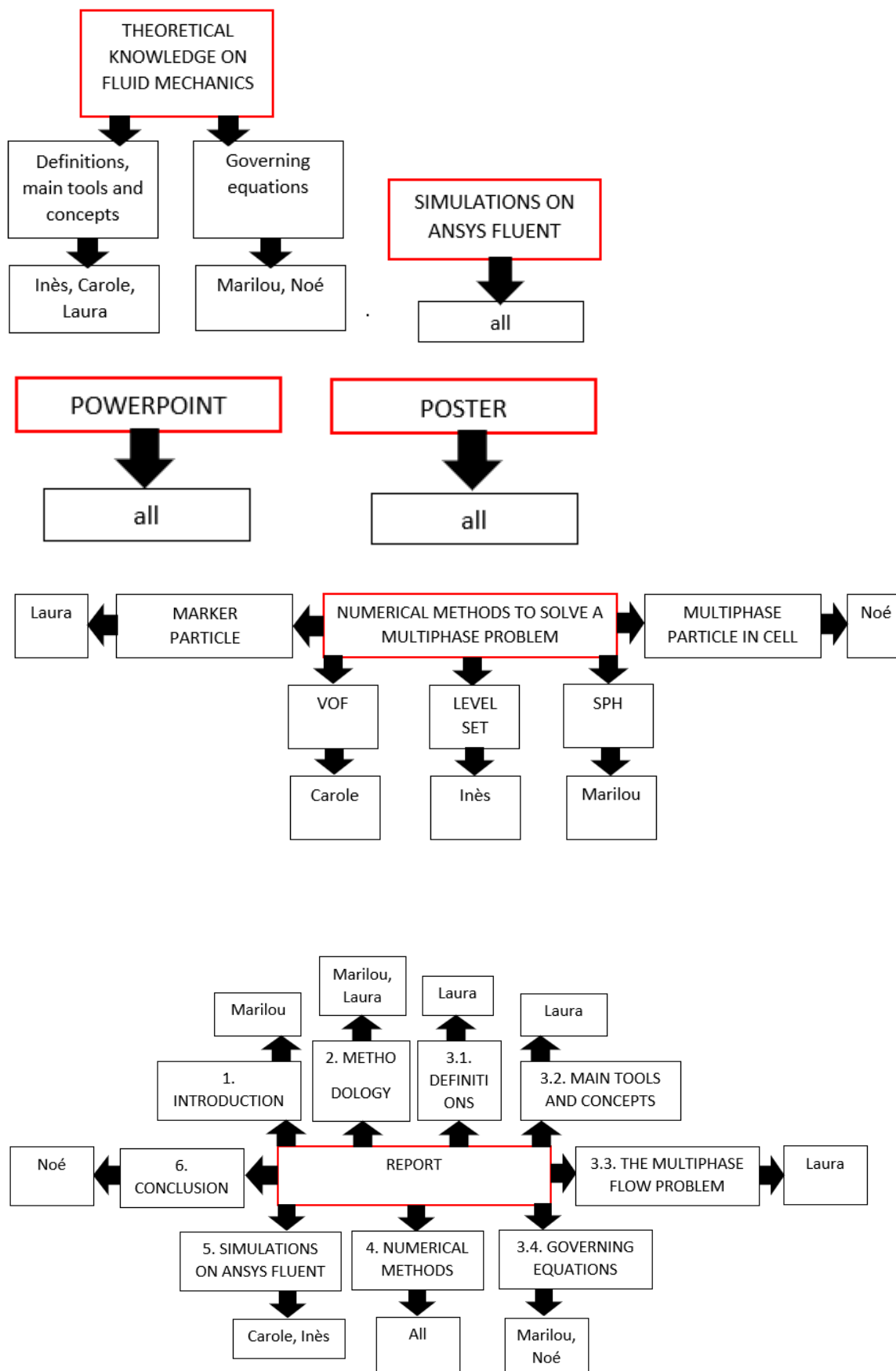
First, we did research on fluid mechanics and multiphase systems. We relied on the book "Fluid mechanics 7th edition", by Franck M.White. We also did some research on the Internet. We pooled our research by adding it to a shared slideshow. Every week, we updated it to show our tutor the progress of our research.

After that, Mr SHADLOO provided us with video lessons to watch. We all watched these to make sure we all had a good understanding of the concepts and of the overall problem.

Then, we did research on the Internet about the numerical methods to solve the multiphase problem.

Once our bibliographic research was completed, we moved on to the simulations on Ansys Fluent. Mr SHADLOO provided us with several explanatory videos on this software then he gave us exercises. Every week, the five of us met at INSA to perform the simulations on Ansys Fluent. Regularly, we called on Zoom to take stock of our project.

The flowchart below details the distribution of the tasks among our group.



3. THEORETICAL KNOWLEDGE ON FLUID MECHANICS

Preliminary remark : in this report, bibliographic sources are marked in square brackets []

3.1. Definitions

- **Fluid mechanics [1]** : it is the study of fluids in motion or at rest, called fluid dynamics and fluid statics. In fluid mechanics there only are two states : fluid and solid. Fluid mechanics has various applications, such as aeronautics, aerospace or the oil industry.
- **Fluid [1]** : Both gases and liquids are classified as fluids. A fluid is a body which flows freely since there is little cohesion between the molecules of which it is composed. The difference between a solid and a fluid resides in the fact that a solid can resist a shear stress (by a static deflection) whereas a fluid cannot. A fluid will move and deform as long as it undergoes a shear stress. The difference between a liquid and a gas relies on the fact that a liquid has a proper volume but not a proper shape, while a gas tends to spread over to occupy all the available space.
- **Turbulent flow [2]** : a type of fluid flow characterized by irregular fluctuations, or mixing. The magnitude and the direction of the flow are both chaotic. The fluid motion undergoes many fluctuations in pressure and velocity. The flow of wind and rivers is generally turbulent. A turbulent flow is the opposite of a laminar flow, which flows smoothly, in paths or parallel layers.

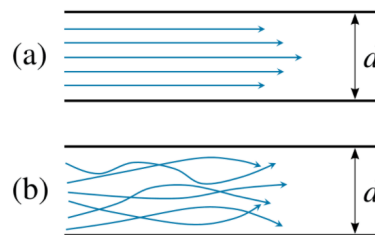


Figure 1 - Laminar (a) versus Turbulent (b) flow

<https://www.simscale.com/docs/simwiki/cfd-computational-fluid-dynamics/what-is-laminar-flow/>

- **Multiphase flow [1]**: it is a flow that contains two (or more) distinct phases that have one or more interfaces in common. Hereinafter we will consider two-phases systems. There are different types of multiphase systems :
 - 1) one fluid in two different phases (for example liquid water and water vapor coexisting at the boiling temperature of water)
 - 2) two immiscible fluids but both in the same phase (gases mix so here we are talking about two liquids). For example, droplets of oil in liquid water.
 - 3) two different fluids in two different phases

Once we have determined the chemical species and their states, we can again distinguish three categories of multiphase systems [24]:

- 1° separated phases : the 2 phases are separated by a geometrically simple interface
- 2° dispersed phases : the distinction between the two phases is far more complex
- 3° mixed phases : both separated and dispersed phases coexist



Figure 2 - Two different multiphase flow models

<https://www.comsol.com/blogs/modeling-and-simulation-of-multiphase-flow-in-comsol-part-1/>

- The **hydrostatic/shear-free condition [1]** : is said when the velocity of the fluid is 0. One of the consequences of this is the fact that the pressure variation is due only to the weight of the fluid. Furthermore, there is no pressure change in the horizontal direction. However, there is a vertical change in pressure : the pressure increases proportionally to the depth in the fluid, according to the following formula : $P = P_0 + \rho gh$
- **Eulerian** and **Lagrangian** frame of reference [23]: they are two ways to describe and study flow motion. The Eulerian (used in most cases) approach monitors the flow characteristics in a fixed control volume, while the Lagrangian method tracks individual fluid particles as they move in the domain, the coordinate system moves with the flow

3.2. Main tools and concepts

First of all, let's give a reminder of the main thermodynamic properties of a fluid :

Pressure P in Pascal (Pa) or in N/m² is the stress exerted on a unit area of the fluid.

Temperature T in Kelvin (K) or in degrees Celsius °C = K - 273,15

Volumic mass $\rho = \frac{m}{V}$ in kg/m³

Density $d = \frac{\rho}{\rho_0}$ (no dimension). It is constant for a liquid, but for a gas it varies with pressure.

Now let's remind ourselves of the **state relations for gases and liquids [22]** :

State relations for gases :

- Perfect gas-law (high temperatures and low pressures only) :
- $P = \rho RT$ or $PV = nRT$ with $R = c_p - c_v = 8,314 \text{ J/mol.K}$ the universal gas constant
- $c_v = \frac{du}{dT}$ in J/kg/K the molar heat capacity at constant volume
- $c_p = \frac{dh}{dT}$ in J/kg/K the molar heat capacity at constant pressure
- $k(T) = \frac{c_p}{c_v} \geq 1$ kair = 1,4 the specific heat ratio

State relations for liquids :

- Liquids are nearly incompressible
- $\rho = \text{constant}$ $c_p = c_v = \text{constant}$ $dh = c_p dT$

Shear stress $\tau = \frac{F}{A}$ in Pa. With F the tangential force applied and A the area of the section that is tangential to the force.

Viscosity (or dynamic viscosity) [1] is a measure of a fluid's resistance to deformation. It determines the fluid rate that is generated by a given applied shear stress. That is why it is more difficult to move through water than through air, and even more difficult through oil.

$$\mu = \frac{\tau}{\frac{du}{dy}} = \frac{\tau}{\frac{d\theta}{dt}}$$

μ is the coefficient of viscosity in kg/m/s.

It's important to know that viscosity is a function of temperature. That of liquids decreases when the temperature increases. On the contrary, the viscosity of gases increases when the temperature of the system increases.

Kinematic viscosity [6] measures the ability of a fluid to resist to flow when it doesn't undergo any external force, except gravity : $\nu = \mu/\rho$ in m^2/s

Thermal conductivity [8] coefficient k is a parameter that characterizes a given material. k depends on the temperature, the physical properties, the water content, and the pressure of the material. Its unit is the W/m.K. A material that is a heat conductor will have a large k, whereas a material with a low k will be considered as a thermal insulator.

The Reynolds number Re [1]: $Re = \rho VL/\mu = VL/\nu$ where V and L are velocity and length scales of the flow. This number is dimensionless. A low Re means viscous motion, inertia effects are negligible. A moderate Re implies a smoothly varying laminar flow. A high Re means a turbulent flow.

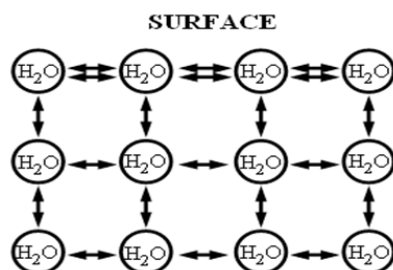


Figure 3 - Representation of the surface tension

Surface tension [4] : Let's consider a liquid in a container. The liquid is in contact with air on its upper side. For example, let's imagine water in a glass. Since it is in a container, the water can not move freely. We know that, in general, the water molecules tend to cling to each other. At the surface of the water, there are fewer water molecules to cling to since there is air above.

To make up for this lack of water molecules, the water creates an interface with the nearest fluid : air. This surface layer is very strong. This is what we call surface tension. It is denoted as σ , in N/m. This phenomenon is responsible for the spherical shape of liquid droplets : the cohesive forces at the interface pull the water towards the center of the droplet.

It is useful to know that when the temperature increases, the surface tension decreases.

Surface tension is also to be taken into account in a multiphase : A liquid, being unable to expand freely, will form an interface with a second liquid or gas.

For a water-air interface at 20°C, $\sigma = 0,073 \text{ N/m}$

The **Capillary number Ca [1]** (or N_c in the oil industry) :

For a liquid (single phase) in contact with air : $Ca = \frac{\mu V}{\sigma}$ For a multiphase : $Ca = \frac{\mu V \mu'}{\sigma \mu'}$

Where μ is the viscosity of the continuous phase, μ' is the viscosity of the dispersed phase, V is the velocity and σ is the surface tension. This number is dimensionless. Let's consider an interface between a liquid and a gas or between two fluids that are immiscible. Ca represents the effect of viscous drag forces relatively to the surface tension forces across this interface. For example, an air bubble in a liquid flow tends to deform because of the viscosity. But at the same time, surface tension minimizes the surface area. Ca enables us to compare these two phenomena.

Internal energy U (in J) [22] : it is the sum of the kinetic energy and the potential energy of the system. The kinetic energy is due to the motion of molecules. The potential energy is the result of the vibrational motion and electric energy of atoms.

For a closed system $\Delta U = Q + W$

Where ΔU is the change in internal energy of a system during a process, Q is the heat and W is the mechanical work.

Enthalpy H (in J) [22] : it is defined as $H = U + PV$

Entropy S (in J/K) [22] : it is a measure of the microscopic disorder of a system. Please look at the 2nd law of thermodynamics for its definition.

And finally, let's give the two laws of **thermodynamics** :

First law of thermodynamics (conservation of energy) [22]:

Let's consider a closed system. The energy variation of the system depends only on the energy transfers between the system and its external environment :

$$E_2 - E_1 = W_{1 \rightarrow 2} + Q_{1 \rightarrow 2}$$

with $Q_{1 \rightarrow 2}$ the amount of heat supplied to the system between states 1 and 2, $W_{1 \rightarrow 2}$ the mechanical work supplied by the system and E the energy of the system.

Second law of thermodynamics (entropy) [22]:

The entropy variation of a system during a transformation is :

$S_f - S_i = S_{i \rightarrow f}^e + S_{i \rightarrow f}^c$ with $S_{i \rightarrow f}^e = \frac{Q_{i \rightarrow f}}{T_{ext}}$ the entropy exchanged between the system and the external environment ($Q_{i \rightarrow f}$ is the amount of heat exchanged between the system and the external environment). And where $S_{i \rightarrow f}^c$ is the entropy created. It is zero if the transformation is reversible. If the transformation is adiabatic (no heat exchange with the exterior), there is no entropy exchanged.

3.3. The multiphase flow problem

Why is it difficult to solve a multiphase flow problem ? [1]

In a multiphase system, each phase has its own volume fraction, its own properties, its own speed and temperature.

Let's consider the water vapor/liquid water biphased system, which is probably the most frequent in the industry, for example in steam generators and condensers. The density of liquid water at 0°C is 997 kg/m³ while that of steam is 916,8 kg/m³. As a result, the influence of gravity on a multiphase flow is different (it is more important) than the influence of gravity on a single phase flow. The different densities and viscosities of the coexisting fluids make multiphase flow more complicated to study than a single-phase flow. Moreover, heat transfer and mass transfer can occur between the different phases, which makes it more difficult to predict the behavior of a multiphase flow.

In addition, surface tension has to be considered in a multiphase flow problem, which makes it more complicated to study than a single phase problem. The interface is very important in multiphase flows. Indeed, that is where the phase changes. A heat transfer, and a momentum exchange can also occur at the interface.

What methodology do we use to solve a multiphase flow problem ?

Methodology for analytical solving[1] :

- Make sure that you **understand the problem correctly**, you have to know exactly what problem you want to solve.
- **Collect the properties** defining your different phases. What do you know about the phases ? Maybe you know which state they're in, their density, viscosity, is it steady or not, do the pressure changes have to be taken into account or not...
- **Choose the adequate model** : For example, what kind of multiphase flow are you considering ? separated, dispersed, mixed phases ?
- Maybe **do a drawing** to get a clearer view of the problem
- **Solve the problem**. In all cases, a fluid flow must satisfy the three basis laws of mechanics plus a thermodynamic state relation and associated boundary condition :

- Conservation of mass (continuity)
- Linear momentum (Newton's second law)
- First law of thermodynamics (conservation of energy)
- A state relation like $p=p(p,T)$

There might be other equations that you want to solve depending on the problem. Apply the adequate boundary conditions at solid surfaces, interfaces, inlets...

- **Give a numerical result** that is as precise as possible and in the adequate units.
- **Comment on your result**, compare it to your initial hypotheses, tell whether or not it is precise, discuss the hypotheses that you used to simplify the problem.

Methodology for numerical solving (using Ansys Fluent) [videos sent by Mr Shadloo] :

- **Create a 2D or 3D mesh** using Ansys WorkBench
- **Set up the domain** : define the quality, size, geometry, units of your domain. You can also do different hypotheses, for example : is your problem steady ? Does gravity have an influence on your problem ? Activate the adequate equations, such as the energy equation for example, depending on your problem.
- **Set up physics** : Select the multiphase model. Select options such as steady state problem, pressure-based, density-based, multiphase, laminar or turbulent... Choose the adequate materials for your phases. Choose cell zone conditions and boundary conditions. Patch your first phase to add the second phase in it. Define "User defined function (UDF)" : for example to implement specific boundary conditions or specific functions
- **Solve the problem** : Choose the control parameters, initialize the problem, select the number of iterations and then run the calculation.
- **Post Processing** : Now that the solving is done, we want to see the influence of the resolution of the mesh, of the time step size, of the number of iterations... Therefore, we have to change one parameter and then do the same simulation again. if the results are converging, that means that the results are mesh independent (or delta t independent...etc)

How do we choose between analytical solving and numerical solving ? What are their advantages and disadvantages ?

Analytical methods have been used for much longer than numerical methods. However, analytical methods have several drawbacks :

They are quite **long** and **difficult** to implement. Furthermore, they can be quite **imprecise**. Indeed, to solve a problem analytically, we often have to do hypotheses and approximations.

On the contrary, numerical methods are **quick** and **easy** to implement (if we assume that one knows how to use Ansys Fluent). Secondly, numerical methods make it possible to obtain precise results.

In addition, a machine is often more efficient than a human who can make miscalculations. Numerical methods also offer **visual results** (you can do animations on Ansys Fluent, see hereinafter the inkjet problem for example). These visual results are often **easier to understand** than the values that you would obtain with the analytical solving. All the more, analytical results often come hand in hand with lab experiences, in order to have a real life visualization of the results obtained analytically. But these lab experiences are often expensive and the measuring devices aren't always precise. Conversely, numerical simulations are quite cheap and very precise. Finally, numerical methods make it possible to study problems that have to do with the industry. In the industry, facilities are large and sometimes present hazards. Thus, it is easier to carry out numerical simulations rather than to go on site to study them.

3.4. Governing equations [1], [27]

Fluid mechanics is governed by a certain number of equations. Most of them are complicated and involve a lot of variables and computations, that is why we need to apply some and solve them numerically. Some of them are applications of known equations used for solid mechanics and some others concern new properties of fluids. In this section we are going to present to you the main equations that are used in fluid mechanics and their context. The analysis of a fluid flow using these equations is always done on an infinitesimal region of the fluid. It is a differential analysis, we use a control volume to derive the basic equations of mass, momentum and energy. By doing this we are able to solve all equations in any given fluid mechanics problem, using the thermodynamic laws we recalled earlier and provided with boundary conditions. All the equations that you will see in this part are described using the following cartesian vector form of the velocity field :

$$\vec{V}(r, t) = u(x, y, z, t) \vec{i} + v(x, y, z, t) \vec{j} + w(x, y, z, t) \vec{k}$$

The equations are also in the Eulerian frame of reference except if mentioned otherwise.

There are three main differential equations in fluid mechanics, they are called the Navier Stokes equations. If the viscous effects are negligible, they can be simplified to give first order equations that are called the Euler equations. The first one is the differential equation of mass conservation, also called the equation of continuity. For it to be used, we need two assumptions. The density and the velocity field need to be continuous functions. It is the following in the general form (It also has a specific form for steady compressible and incompressible flow(1)):

$$\frac{\partial \rho}{\partial t} + \text{div}(\rho V) = 0$$

The second one is quite complex, it is the differential equation of linear momentum. It is the result of the application of Newton's Second Law of motion to the control volume. We obtain three components with τ the viscous stress tensor acting on the element :

$$\rho g_x - \frac{\partial p}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} = \rho \left(\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} \right)$$

$$\rho g_y - \frac{\partial p}{\partial y} + \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{zy}}{\partial z} = \rho \left(\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} \right)$$

$$\rho g_z - \frac{\partial p}{\partial z} + \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} = \rho \left(\frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} \right)$$

Finally, the third equation is the differential equation of energy. It is obtained by applying the first law of thermodynamics to the control volume. It has the following form, where Φ is the viscous dissipation (the conversion of fluid energy into heat through friction)

$$\rho \frac{du}{dt} + P(\nabla \cdot V) = \nabla \cdot (k\nabla T) + \Phi$$

In addition to these differential equations, there are other functions that help describe a fluid's behaviour. First of all there is the stream function. This function allows to satisfy the continuity equation and to solve the momentum equation using a single variable Ψ . It can be used when the continuity equation can be reduced to only terms, we obtain the following definition :

$$u = \frac{\partial \psi}{\partial y} \quad \text{and} \quad v = -\frac{\partial \psi}{\partial x}$$

Other concepts that are useful in analyzing fluid flow problems are vorticity and irrotationality. The vorticity describes the local spinning of a particle as it goes along with the flow, flows that have negligible or no vorticity are irrotational. Mathematically, it is twice the mean angular velocity vector of the particle, also described as the curl of the flow velocity.

$$\zeta = \text{curl } V$$

The hydrostatic (also called shear-free) condition happens when the fluid velocity is null. Thus, the pressure variation is only due to the weight of the fluid. Under this condition [1], [23] :

Pressure gradient or any other stress gradient causes a net force on a fluid when it varies spatially :

$$dF_{press} = \left(-i \frac{\partial p}{\partial x} - j \frac{\partial p}{\partial y} - k \frac{\partial p}{\partial z} \right) dx dy dz \quad F_{press} = -\nabla p = -i \frac{\partial p}{\partial x} - j \frac{\partial p}{\partial y} - k \frac{\partial p}{\partial z}$$

The pressure gradient is a surface force. There may also be a body force due to electromagnetic or gravitational potentials.

$$dF_{grav} = \rho g dx dy dz \quad F_{grav} = \rho g$$

In addition to gravity, a fluid in motion has surface forces due to viscous stresses. By Newton's law :

$$\sum f = f_{press} + f_{grav} + f_{visc} = -\nabla p + \rho g + f_{visc} = \rho a$$

-For hydrostatics, the viscous stresses and the acceleration are zero.

-If the fluid is at rest or at constant velocity : $\nabla p = \rho g$

-The equation for a fluid at rest or at constant velocity and the solution to the hydrostatic problem is :

$$p_2 - p_1 = - \int_1^2 \gamma dz$$

-Liquids are nearly incompressible so we can neglect their density variation in hydrostatics.

Thus $p_2 - p_1 = \gamma(z_2 - z_1)$ where γ is the specific weight of the liquid.

Gases are compressible, with density proportional to pressure. Thus density must be considered as a variable. Perfect-gas law : $p = \rho RT$

$$\frac{dp}{dz} = -\rho g = -\frac{pg}{RT} \qquad \frac{dp}{p} = -\frac{gdz}{RT}$$

After an integration between 1 and 2 and using the approximation of the isothermal atmosphere, (where $T=T_0$, the sea-level temperature)

$$p_2 = p_1 \exp \left[-\frac{g(z_2 - z_1)}{RT_0} \right]$$

Euler's theorem [23] : $\sum \vec{F}_S + \sum \vec{F}_V = \int \int_S \rho(\vec{U} \cdot \vec{n}) \vec{U} dS$

where $\sum \vec{F}_S$ is the sum of the pressure forces and $\sum \vec{F}_V$ is the sum of the volume forces

Bernoulli's equation [23] : This equation is really important in fluid mechanics, it can be applied only under conditions : the flow must be incompressible and stationary. The forces must be conservative. The fluid should be perfect (not viscous) et we apply the equation along a current line :

$$d\left(\frac{U^2}{2} + \frac{p}{\rho} + gz\right) = 0 \text{ or also expressed } \frac{U^2}{2} + \frac{p}{\rho} + gz = \text{constant}$$

$F_v = \text{grad}(P) = \rho f_v$ The relation between volume forces and pressure

$d\vec{F}(N) = -P(N)dS\vec{n}$ The expression of a pressure force over a surface element dS , with the normal vector oriented towards the exterior.

4. NUMERICAL METHODS TO SOLVE A MULTIPHASE PROBLEM

The problem is : how to track the location of the interface in a multiphased system ?

The different methods available use different types of coordinate systems. Some use the Lagrangian frame of reference, some the Eulerian, and some use a mixed frame of reference that employ both systems.

There are two types of methods that we can use for interface modelling :

- 1) Interface **tracking** : the interface is generated by tracking fluid trajectories in a Lagrangian field (or mixed Eulerian-Lagrangian). For instance, the Level Set method is based on interface tracking.
- 2) Interface **capturing** methods : the interface is constructed thanks to the fluid properties. For instance, the VOF method is based on interface capturing (the fluid property that is used is the volume fraction).

A key element to the understanding of numerical simulations is the mesh. A mesh is a representation of a larger domain using smaller discrete cells. It allows the solving of differential equations on a unique, small element, where we are unable to solve on the whole domain. After doing so we can do an approximation of the solution on the larger domain. There are different types of meshes, some may be structured and regular, others may not. We can also encounter hybrid types of meshes. In the same way, the cells may vary from one mesh to the other, there are cells that are triangular or quadrilateral. The utility of different forms lies in the simplification of the solving process, and the choice and creation of the mesh is a key step in a numerical analysis.

4.1. SPH method [24]

The Smoothed Particle Hydrodynamics (SPH) is distinguished from the others by the fact that it is a meshfree method. It is a Lagrangian method where the idea is to model a continuous fluid by discretizing it by a series of points whose mass is constant. It means that we consider the flow to be represented by replacing the mesh with a finite number of particles that carry the fluid characteristics properties (position, velocity, mass ...). Its advantages are numerous : the fact that it is meshless simplifies the implementation of the model and it can be extended to a lot of domains. The simulations also have a really low cost by number of particles compared to the method with meshing, when the metric of interest is related to fluid density. The limitations of this method are the difficulty of setting boundary conditions, and the lack of accuracy on the whole domain. Because of this, SPH methods are often used in real-time animation and video games where accuracy is not as important as interactivity.

The key element of this method consists of a kernel function that describes the interaction between particles. This function is used to estimate the values of the physical quantity of a particle by summing the weighted average of neighbouring particles hence the "smoothing". The characteristic radius of this operation or smoothing length, can be fixed in space and time, however SPH can be much more efficient. Indeed, the resolution of the simulation can be made to adapt itself according to local conditions if each particle is allowed to have its own smoothing length that varies with time.

This will create regions where the smoothing length is higher because the density is low, and vice versa, which will improve the simulation by using the computational power in the regions of interest.

4.2. VOF method [12]

This is the method that we will be using in our simulations on Ansys Fluent. The VOF method is a surface-tracking method. It relies on a presence rate function, denoted as C (indicator or colour function). This presence rate function C takes values between 0 and 1 for phase k. If it is 0 or 1, the volume contains only one of the two fluids. If its value is between these two terminals, the volume contains a diphasic mixture and therefore the interface is present.

First of all, we consider the flow of a diphasic medium without phase exchanges. It is described by the volume fraction C of one of the phases, also called the void fraction or colour fonction.

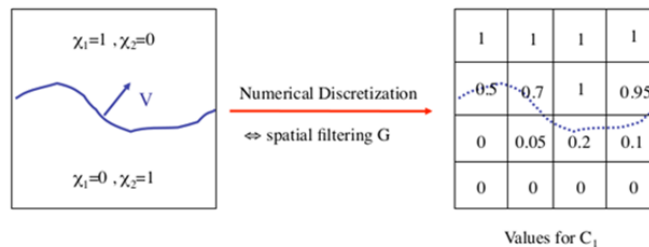


Figure 4 - VOF Discretization

C_{ij} is the portion of the cell i,j that is filled with liquid phase and χ is the phase function :

$$C_{i,j} h^2 \approx \int \int_{i,j} \chi(x, y) dx dy$$

Then we solve the following equations :

$$\frac{\partial C}{\partial t} + U \cdot \nabla C = 0$$

The 3D Navier Stokes equations for an incompressible flow :

$$\nabla \cdot (U) = 0 \quad \rho \left[\frac{\partial U}{\partial t} + \nabla \cdot (UU) \right] = -\nabla p + \mu \nabla^2 U + F$$

where F is the result of the interactions between the phases :

$$F = \sigma \nabla \cdot n \nabla C$$

where σ is the surface tension and n the vector that is normal to the interface.

Note that the volumic mass and the viscosity depend on the function C :

$$\rho = \rho_1 C + \rho_2 (1 - C) \quad \mu = \frac{1}{\rho} [\rho_1 C \mu_1 + \rho_2 (1 - C) \mu_2]$$

Then, it is necessary to reconstruct the interface thanks to one of the two following methods :

- the SLIC method (Simple line interface calculation) : the interfaces are lined up with meshes
- the PLIC method (Piecewise linear interface calculation) based on the local slope but a discontinuous interface

4.3. Level Set method

The level set method is a numerical technique for tracking interfaces. To do so, we introduce a scalar function $\phi(x,y)$ whose zero level set is the interface that we want to describe. The level set function can be seen as various iso-contour and each iso-contour is defined by a set of points at the same length from the interface. Therefore, the sign of the function (+ or -) enables us to know on which side of the interface is the point that we are looking at.[12]

This method tracks the evolution of $\phi(x,y)$ and determines the zero level set thanks to these equations :

$$\phi_t + F|\nabla\phi| = 0 \qquad \frac{\partial\phi}{\partial t} + V \cdot \nabla\phi = 0$$

[25]

Here are some graphics of examples of results that you could obtain with this method :

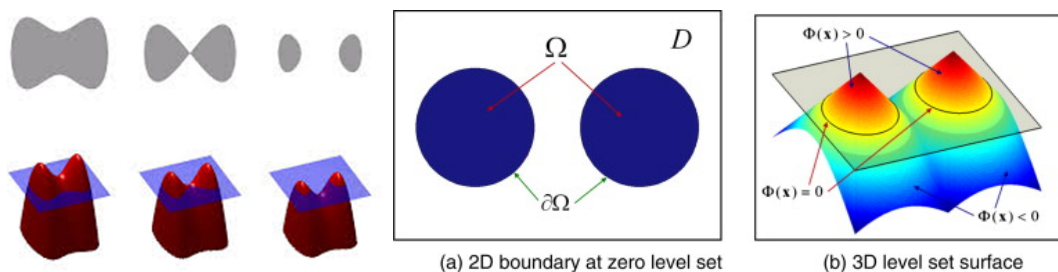


Figure 5 - Different results obtained with the level set method

This method is a great tool for modeling time-varying objects and works in any dimension. However, it does not guarantee conservation of the volume.

4.4. Marker particle method [17]

To explain this method as clearly as possible, we decided to explain it with successive steps :

1. Define a mesh made up of computational cells with centres (x_i, y_j) , initialize at $t=0$
2. Within each cell, assign a set of particles with a total number N in the domain. The particles act as markers, located at position (x_i, y_j) and at a certain t
3. Assign an initial particle colour C_p^m for each fluid : $C_p^m = 1$ if particle p is located in fluid m , or $= 0$ otherwise

4. Construct initial grid cell volume fractions $C_{ij}^{m,0}$
5. For $t>0$: Interpolate velocities to all particles from the nearest 4 grid velocities
6. Solve the equation of motion $u=dx/dt$ using the predictor-corrector strategy
7. Interpolate the new grid volume fractions for each fluid m at the time step $n+1$
8. Update density and viscosity using the new volume fractions.
9. Store old particle positions and particle colour. Increment the time and go to step 1.

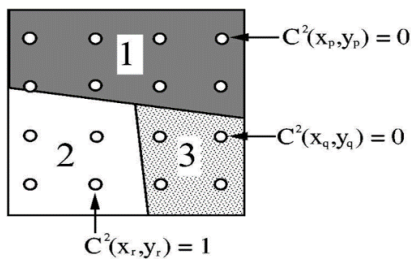


Figure 7 - Results obtained with the 2D marker method

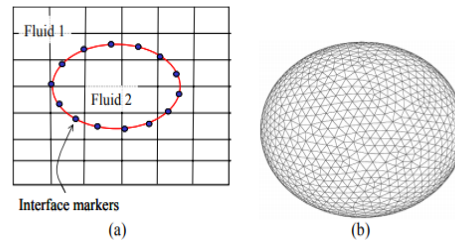


Figure 8 - Results obtained with the 3D marker method

http://etd.fcla.edu/UF/UFE0015703/singh_r.pdf

4.5. Particle in cell method [21]

In the Multiphase Particle in cell (MP-PIC) approach, the particle properties are mapped from the Lagrangian coordinates to an Eulerian grid by using interpolation functions. After evaluation of the continuum derivative terms, the particle properties are mapped back to the individual particles. Even if we did not use this method to solve our problems, it is still really efficient and useful for dense fluid flow. However, we will not go into that much details

The MP-PIC method is described by the following components :

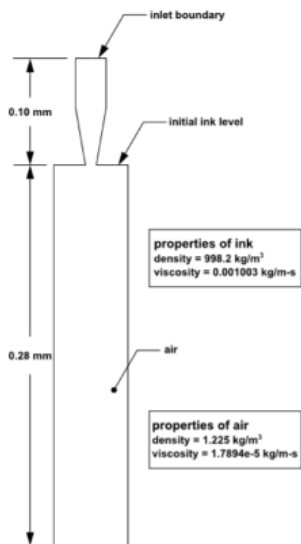
- Governing Equations for the two present phases : fluid and particle, as well as identities of the particle probability distribution function ϕ which is a function that indicates the probability of finding a particle of given properties (velocity, density, volume) at a given time and location. And a coupling of the fluid and particle phase through the particle acceleration.
- Interpolation functions that are used to transfer the particle properties between the Lagrangian particle space and the Eulerian grid. If we assume a grid made of rectangular cuboid cells, the scalar particle properties are inserted to the cell centers meanwhile, the vector properties are interpolated to the cell faces.
- The particle stress model which is a function used to modelize the effect of particle packing

This method has two main limitations : Firstly, all the particles are assumed to be perfectly spherical. Corrections can be made but in case of highly non spherical particles, the interactions may not be well represented. Secondly, the size of the particles has to be small compared to the size of the grid for an accurate interpolation.

5. NUMERICAL SIMULATIONS ON ANSYS FLUENT

5.1. Inkjet Problem

In this experiment, we had to follow a tutorial made by M.Shadloo to determine the ink flux when the ink is ejected by an ink-jet printer. In this simulation, we use a VOF method to solve the problem. The video shows us how to solve the problem step by step after the meshing part. So we had to go in the solver, put the right boundary and initial conditions of the domain and define the interface between the two fluids to be able to examine the flux. Thanks to Ansys Fluent and its multiphase modeling, we were able to define the shape and the movement of the droplets in the air-chamber.



The first step consisted in importing the mesh that our professor gave us.



Figure 10 - Mesh of the inkjet

Figure 9 - Schematic of the Inkjet problem.

We checked the quality of the mesh : it is very close to 1, which is really good.

```
Mesh Quality:
Minimum Orthogonal Quality = 9.93025e-01 cell 6615 on zone 1 (ID: 24600 on partition: 1) at location ( 9.97074e+01 8.73394e+00)
(To improve Orthogonal quality , use "Inverse Orthogonal Quality" in Fluent Meshing,
where Inverse Orthogonal Quality = 1 - Orthogonal Quality)
Maximum Aspect Ratio = 3.65205e+00 cell 8139 on zone 1 (ID: 6860 on partition: 0) at location ( 3.79078e+02 2.65875e+01)
```

Then, we could start to select the right parameters. Indeed, without the correct parameters, we can't obtain a precise simulation. First of all, we had to set up the scale and choose the right units. Then we defined the nature of the different fluids (the air and then the ink which had the same properties as the liquid-water in our problem) and finally, the boundary conditions. In order to set the boundary conditions as a function of time, we used a function UDF already defined and given by our professor to make it easier for us to interpret. We then patched the domain : the main domain contains air, with an inlet of ink.

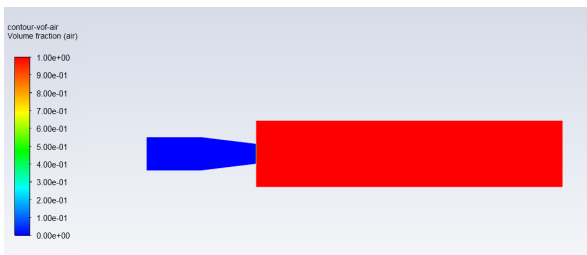


Figure 11 - initial patching of the domain

In this problem, we choose a pressure based simulation. So, we set the parameters in order to see this evolution at the end of the resolution. As said before, we choose a VOF method, therefore the phases are in eulerian type, the time is transitory and we put the absolute velocity. Next, we had to solve the problem, here is a view of the results that we obtained.

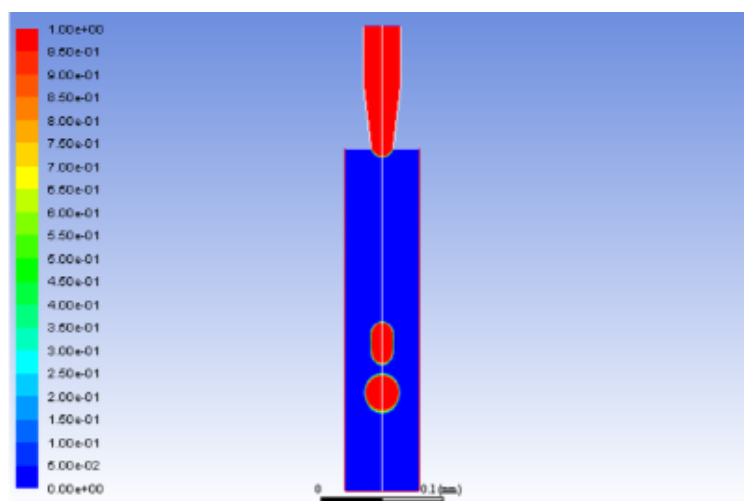


Figure 12 -The result of the simulation (contours of VOF)

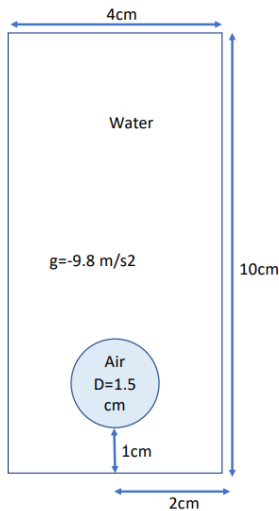
As we can see on the picture, after the calculations, we observe the variation of the position and the shape of the interface between the two fluids.

We can see that the two bubbles of ink deform and move vertically from the inlet straight to the opposite wall of the domain. It is important to mention that in this problem, the two main bubbles stay whole (there are no smaller bubbles that detach from the main ones). This is desirable in many applications where you want to separate the two immiscible phases (this will be the case for the next simulation). However, for this inkjet problem, if smaller bubbles had detached, it wouldn't have been a problem.

5.2. Oil bubble in liquid water

The problem that we want to solve is the following : in the petroleum industry, when oil is extracted from a well, water is often injected under pressure into the reservoir. This increases the pressure in the reservoir, which allows more oil to be withdrawn. This method therefore aims to increase productivity. However, this implies that the oil is in the presence of water, with which it is immiscible. These two phases must then be separated. This separation takes place on site because moving the total volume would be too expensive. The objective of our simulation is therefore to model the behavior of a drop of oil in water.

Our simulation should present a bubble which, by its density lower than that of water, should rise to the surface of the water and deform during this rise. For a practical matter, we replaced in our simulation the oil bubble by an air bubble, because the lower viscosity of the air allows us to observe results more quickly, after less iterations. However, the behavior of an oil bubble in water would be quite similar, we would just have to change the viscosity.



First of all, we made the geometry : We chose an element size of $5,0e-4$ m. The mesh quality is very close to 1, which is very good.

Then we assigned the proper materials to our first phase (water).

We set the value for the surface tension at 0.072 n/m and the following boundary conditions : contact angles at 90° and no slip for the shear condition. We also set the only force exerted on the bubble of air : gravity, in the y direction, whose value is $9,81\text{m/s}^2$. For the solving we used the fractional step scheme. We designed an air bubble and then patched the water phase with this bubble. We put the screenshots of all selected parameters in Ansys Fluent in the annexes.

Figure 13- Schematic of the problem

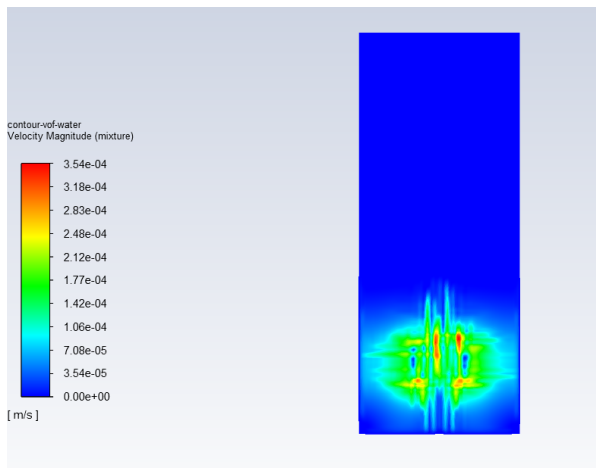


Figure 14 - Initial velocity magnitude

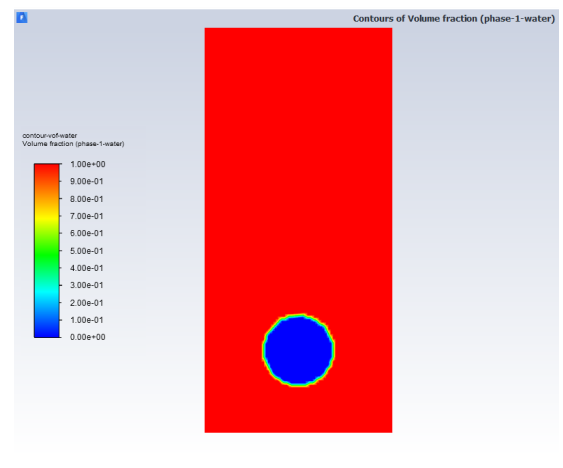


Figure 15 - Initial contours of volume fraction

First we did the solving for 12,000 time steps, with a time step size of $1e-4$ s.

We tracked the evolution of the VOF and of the velocity :

Hereinafter we are giving a few images of the evolution of the contours of VOF. To see more of them, please refer to the annexes.

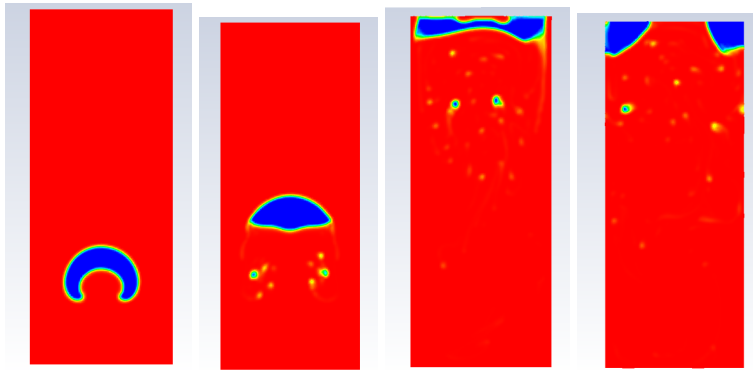


Figure 16 - Results of the simulation of the bubble of air in water of the first mesh (contour of VOF)

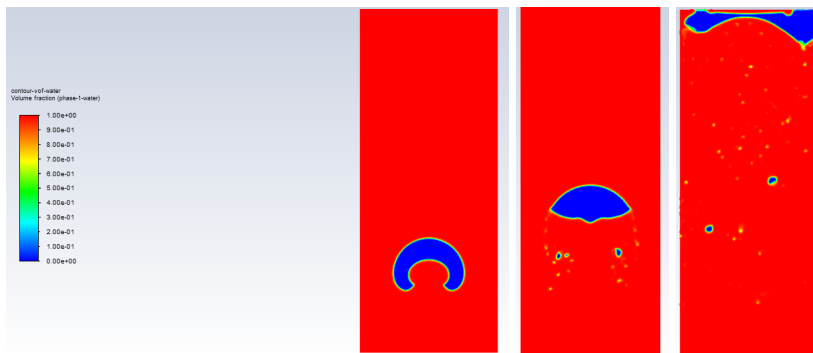


Figure 17 - Results of the simulation of the bubble of air in water of the second mesh (contour of VOF)

We can see that the bubble starts by deforming, then takes the shape of a downwards oriented croissant. The tips of the croissant finally detach from the rest of the croissant. The main "bubble" of air continues to go up since its density is lower than that of water. As the time goes by, smaller bubbles detach from the main one. We can also see that these smaller bubbles that have detached start to move in a circular movement through the water phase. It is important to mention that the fact that smaller bubbles detach is not desirable since what we want to do in the first place is to separate the two phases from one another. As a result, it would be more convenient to keep the second phase as a single bubble of oil. However, in a previous problem (inkjet problem) the fact that smaller bubbles detach would not have been a problem, it could even have been convenient for the printing.

Afterwards, the main bubble arrives at the top of the water phase. It splits into two and each part goes to one upper corner of the box.

Finally, the two parts of the bubble reunite and the bubble "floats" at the surface of water. The two phases are now perfectly distinct.

Secondly, we moved on to post-processing. We wanted to see the influence of the mesh resolution, so we duplicated our mesh and assigned the following resolution :

Initial mesh :

- element size = 5,0e-4m
- Number of elements = 15439
- Number of nodes = 15704

Second mesh :

- element size = 5,0e-3m
- Number of elements = 160
- Number of nodes = 189

We did the solving again with this second mesh (still 12000 time steps with a step size of $1e-4s$). We can see from the previous screen savings that the results are converging. We can conclude that the result is mesh independent.

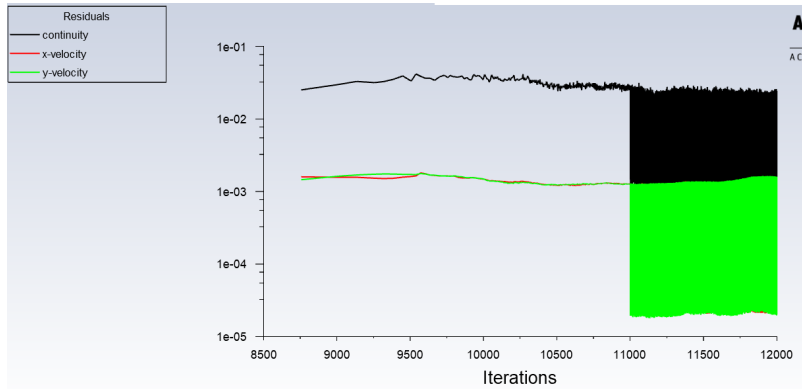


Figure 18 - Scaled residuals (element size of $5e-4m$)

We did a second solving, in which we tracked the evolution of the velocity magnitude :

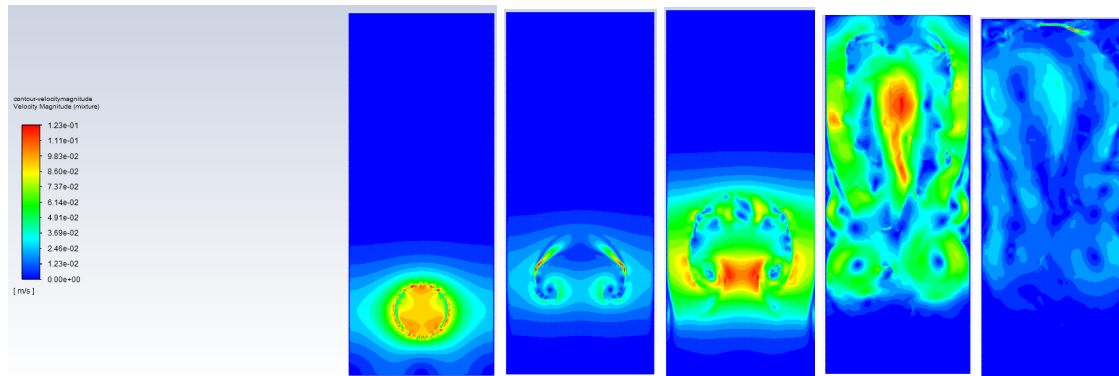


Figure 19 - Results of the simulation of the contours of velocity

In the initial state, the velocity is high only around the air bubble, because it is near the interface between the two phases. The velocity inside the bubble is higher because air is less dense than water so the forces applied on this phase have more impact on its velocity.

Then, when the bubble's shape changes, there are two rotation points that lead to the creation of smaller bubbles and we can see that the velocity is higher around those two points.

Afterwards, the bubble starts to move towards the top of the box, as the water flows on the sides of the bubble because of gravity and reaches its maximum speed when reaching the bottom of the bubble, we observe that the highest magnitude of the velocity is always just under the bubble.

Even when the air has reached the top, the water stays agitated for a while on the path followed by the bubble (as shown on the rightest picture in Figure 19)

To finish, we wanted to see the influence of the time step size on the results of the contours of VOF. For this purpose, we increased the time step size from $1e-4s$ to $5e-5s$ and ran the calculation of the contours of VOF over again.

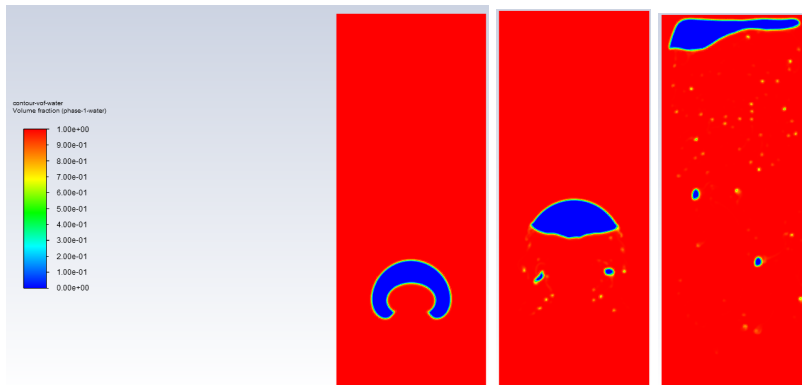


Figure 20 - Results of the simulation of the contours of VOF with a different time step size ($5e-5s$)

We can see that once again the results converge. We can conclude that the result is independent from the time step size.

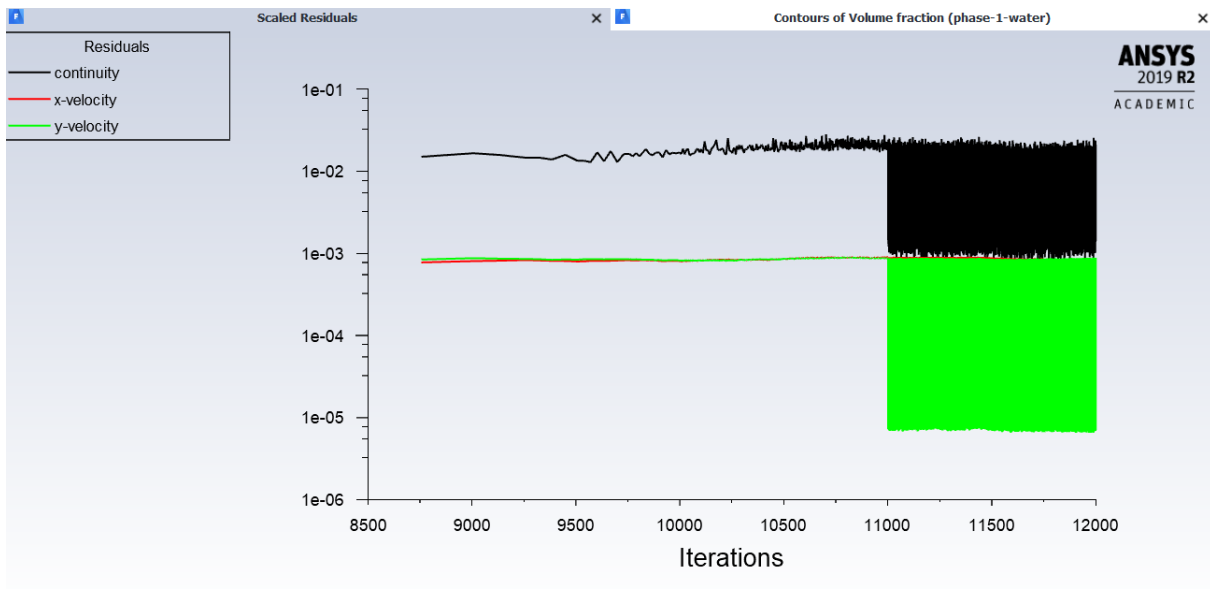


Figure 21 - scaled residuals with the different time step size ($5e-5s$)

6. CONCLUSION AND PERSPECTIVES

This project has been very enriching for us, academically, professionally and personally.

First of all, this project allowed us to deepen our knowledge of fluid mechanics. Numerical simulations have allowed us to supplement the teachings received in P8 with a practical approach: they allow a visual interpretation of a scientific problem that is initially theoretical.

In addition, our project dealt with an industrial issue: the separation of oil and water in the oil industry. We have enjoyed working on such a concrete issue.

In addition, we had to write a report in English, hold scientific discussions in English and read scientific journals in English. By doing so, we were able to use English in a professional setting (excluding English lessons). This will probably be useful in our professional life.

Finally, the group work has given us a lot. We all got along very well and the organization was spontaneous. We would also like to thank Mr SHADLOO for his help and kindness throughout the course of our project.

One way to continue our project would be to study other types of multiphase systems, perhaps with applications in other industries. In addition, we could use numerical methods other than the VOF method. Thus, we may be able to compare these methods with each other.

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8. ANNEXES :

Array comparing the numerical methods :

During our project, we only used the VOF method for our simulations on Ansys Fluent. However, if we were to use these methods someday, it would be interesting to know their advantages and disadvantages. We decided to compare the VOF method that we used to Lagrangian, Eulerian-Lagrangian methods and to the Level Set method (which can be coupled to the VOF on Ansys). We found the following array online, on https://www.researchgate.net/publication/234446675_Three-dimensional_marker-based_multiphase_flow_computation_using_adaptive_Cartesian_grid_techniques :

Methods	Advantages	Issues
Lagrangian	The interface is known explicitly known and it is part of the computational grid The geometric properties are directly computed on the interface	The method requires to regenerate the grid quite often This method is difficult and expensive for complex 3D problems
Eulerian (eg level set)	The geometric computation is easy All the computations are done on the Eulerian grid The topology changes are easy to handle	There are significant mass loss or mass gain in certain areas of the interface
Eulerian (eg VOF)	No mass loss/gain All the computations are done on the Eulerian grid The topology changes are easy to handle	The performance is low in certain areas of the interface The geometry computation is difficult
Mixed Eulerian-Lagrangian	The interface is known explicitly All the flow computations are done on the Eulerian grid	The data-structure and book-keeping are difficult for 3D problems It is difficult to handle topology change

Figure 22 : comparison of the numerical methods

Zone Name: surface_body Phase: mixture

Adjacent Cell Zone: box

Momentum Thermal Radiation Species DPM Multiphase UDS Wall Film Potential Structure

Wall Motion

Stationary Wall
 Moving Wall

Motion

Relative to Adjacent Cell Zone

Shear Condition

No Slip
 Specified Shear
 Specularity Coefficient
 Marangoni Stress

Wall Roughness

Roughness Height (cm): 0
Roughness Constant: 0,5

Wall Adhesion

Contact Angles (deg):
phase-2-air phase-1-water 90.00001299439

Figure 23 : boundary conditions for the oil bubble in water simulation

Multiphase Model

Model

Off
 Volume of Fluid
 Mixture
 Eulerian
 Wet Steam

Number of Eulerian Phases: 2

Coupled Level Set + VOF

Level Set

VOF Sub-Models

Open Channel Flow

Volume Fraction Parameters

Formulation

Explicit
 Implicit

Volume Fraction Cutoff: 1e-06
Courant Number: 0.25
Default

Options

Interface Modeling

Type

Sharp
 Sharp/Dispersed
 Dispersed

Interfacial Anti-Diffusion

Expert Options...

Body Force Formulation

Implicit Body Force

OK Cancel Help

Figure 24 : boundary conditions for the oil bubble in water simulation

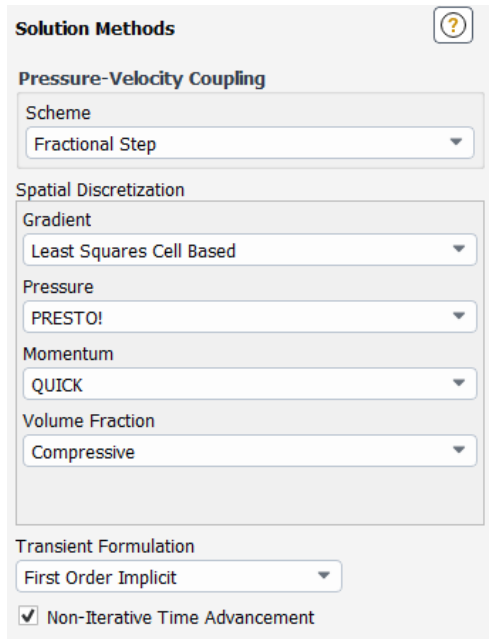


Figure 25 : solution method for the oil bubble in water simulation

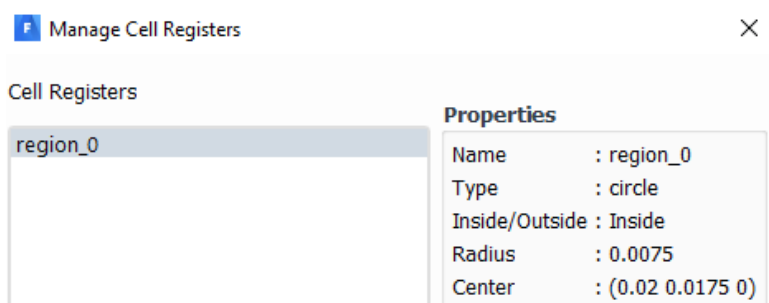


Figure 26 : design of the bubble region for the oil bubble in water simulation