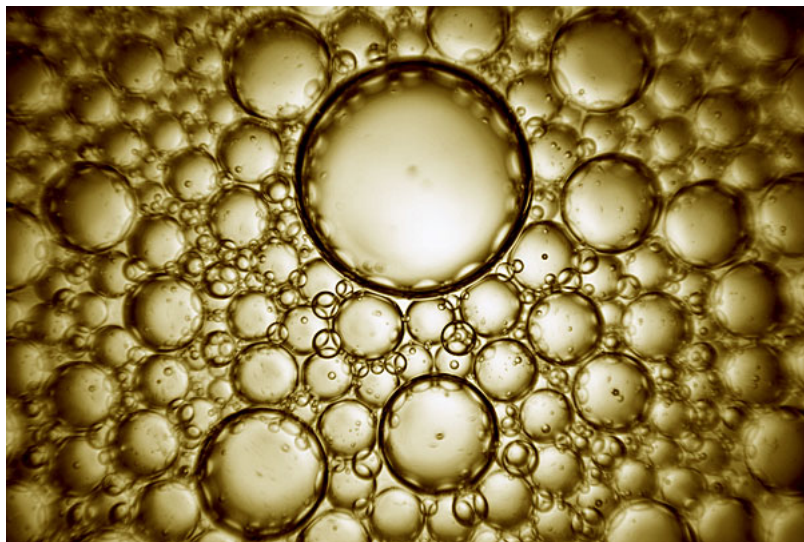# Methods and simulations of water/oil separation in petroleum industries

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Name of project : Methods and simulations of water/oil separation in petroleum industries

Type of project : bibliography and simulations

Objectives of project :
- Understanding the mechanism of water/ oil separation through different methods.
- Visualisation of the behavior of two fluids under multiple conditions.
- Research for the recent works done on the subject (Litterature review).

Key-words : surface tension, Gerris, electrohydrodynamic

Contents

Introduction

The separation of two immiscible fluids is a key element in many domains and in numerous industries. As a matter of fact, water and oil mixtures often need to be separated in order to enhance the productivity of industries. The separation process can be done using multiple methods, each one having its own advantages and drawbacks. Based on the domains of application, industries often use a combination of many of these methods in order to maximize the efficiency of the separation. This process can be found in various domains, such as crude oil extraction where the fluid to remove from is water, or for example in cars' engines where oil has to sometimes be removed from the water. Considering the importance of such a notion, we have decided in our physics' project to deal with the water/oil separation in petroleum industries. Crude oil extraction consists in injecting high pressure water in the oil well in order to get the crude oil at the surface. Therefore, water droplets are emulsioned in the crude oil. The water representing an extra cost of shipping, water droplets have to be removed before shipping the crude oil to the refinery. Many methods exist to remove water from crude oil, they are chosen according to their cost and the feasibility of the implementation next to the oil well. For this project, we have investigated on the techniques employed in water removal. We mainly focused on the electrohydrodynamic method which consists in applying electrical power to the emulsion in order to make the water droplets coalescing. This method involves laws applying to a fluid such as surface tension forces. To visualise these effects, we have done some simulations with the software Gerris.

Part I

Methodology/ Work organisation

Chapter 1

Techniques

An oil water separator (OWS) is a device designed to separate oil from water. Different kinds of separators exist on the market and are used in different industrial areas according to their capability, properties and performance. Indeed, many parameters lead the choice of the oil water separator.

1.1   Hydrocyclone separator

A Hydrocyclone oily water separator is a device designed to separate oil and water. First of all, a hydrocyclone is defined by Wikipedia as a device to classify, separate or sort particles in a liquid suspension based on the ratio of their centripetal force to fluid resistance.

Design: As shown on Figure 1.1.1, the device had two exits on the axis, one on the bottom to reject the unwanted substance, and one on the top to inject the oily water and has no rotating parts. They can be made of metal, ceramic or plastic.
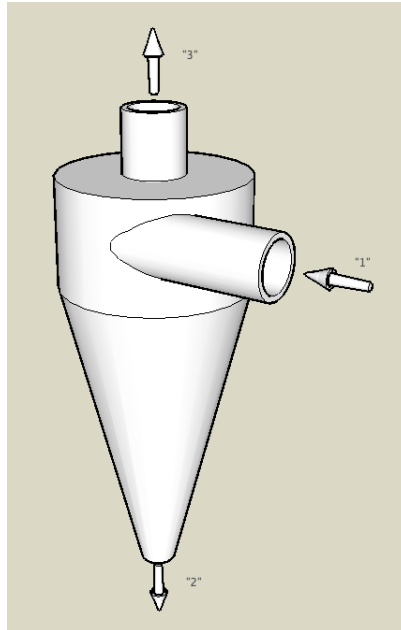
Figure 1.1.1: Diagram of a hydrocyclone: the liquid-solid mixture enters, heavy solids leave, cleaned liquid leave.

It depends mainly on "the characteristics of the feed stream" which includes the density, pulp viscosity, oil concentration and temperature. It includes also "the geometry of the cyclone", which means the shape and dimensions (angles, length, **vortex**...).

Mechanism: First of all, the mixture is injected into the hydrocyclone so that the **vortex** would be created (cf centrifugal separator). Because the two phases have different densities, the centrifugal acceleration would be able to dispatch the two phases. The denser substance (water) will be expelled thanks to the bottom exit. This process is shown on Figure 1.1.2.

Figure 1.1.2: Schema showing centrifugal forces in a hydrocyclone for oily water separation

Advantages: According to "cleanwater", this separation method has many advantages :
   - Removes oil droplets down to 10-15 microns.
   - Low operating costs.
   - Exceed water authority requirements for hydrocarbon discharge.
   - Pre-plumbed and pre-wired.
   - Suitable for use in a wide range of industries.
   - Available upgrades to suit hazardous areas.
   - Lowest maintenance systems on the market.
   - One-off purchase with working life of more than 20 years.
   - Relatively small footprint (compared with traditional separators).
   - Automated and low operating costs.
   - Durable stainless steel construction
   [27, 12]

1.2 Electrostatic separation

Oily water can also be separated by electrostatic grids. Indeed, when an **emulsion**[1] contains a nonconductive liquid (oil) and one conductive (water), is treated by an electrostatic field the following phenomena happen:

---

[1]Mixture of two or more liquids that are normally immiscible (unmixable or unbendable). In an emulsion, one liquid (the dispersed phase) is dispersed in the other (the continuous phase)

- When water droplets are polarized they tend to align with the electric force. Afterwards electric fields tend to gather the droplets and make them **coalesce**[2]

- Attracted to an electrode thanks to a direct current, the water droplet keep being attracted to each other forming larger droplets until eventually they settle by gravity.

- Water droplets that are dispersed in the oil are now treated by an alternative current during half the cycle. Droplets are then relaxed and become spherical. By repeating this, the film of emulsifier is weakened and breaks more easily when the droplets collide.

Electrostatic grids are an effective means of breaking emulsions. The droplets move about rapidly and collide with each other and coalesce. This method has a lot of advantages, but also flaws.

Advantages : This technique is usually used with chemical and heat addition, it is used with reduced temperature which results in fuel economy, reduced problems with scale and corrosion formation and reduced light-end loss. The use of this technique lead to the reduction of emulsion-breaking chemicals use.

Disadvantages: With excess water presence the electrostatic dehydration is shorting/arcing, because there is a tendency toward chaining the formation of a chain of charged water particles—which might form links between the two electrodes, causing short-circuiting. Chaining has been observed in emulsions that contain 4% or less water. If chaining causes excess power consumption, the voltage gradient is too large (i.e., the electrical grids of the electrostatic treater are too close together or the voltage is too high) for the amount of water being handled. The breaking out of solution of small amounts of gas also can create sufficient turbulence to impede sedimentation. [5, 13]

There are many other techniques of water/oil separation not mentionned here, but that can be found in Annex A.

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[2]Second step in demulsification. During coalescence, water droplets fuse or coalesce together to form a larger drop

Chapter 2

Forces applied on fluids

2.1 Surface tension

Surface tension can be defined as the apparent interfacial tensile stress that appears whenever a liquid is in contact with a gas, liquid...At this interface, forces develop in the surface of the liquid and make the surface act like a membrane stretched over the fluid mass. This analogical observation explains several phenomena, like when a steel needle is put gently on the water it will float. This is explained thanks to the development of the tension in the "membrane". Another phenomena concern the small droplets of mercury, who tend to form into spheres when put on a smooth surface because the cohesive forces on the surface keep the molecules on a compact shape.

Figure 2.1.1: Test tube showing cohesive and adhesive forces of a water drop[15]

Like shown on Figure2.1.1, the cohesive forces within the drops are stronger than the adhesive forces between the drops and glass. The surface (**meniscus**)[1] of the mercury liquid confined in a tube has a convex shape because the cohesive forces in liquid mercury tend to draw it into a drop to keep a compact shape.

Now what is cohesive and adhesive forces?

---

[1]Meniscus is the curvature of a liquid's surface within a container such as a graduated cylinder

Cohesive forces   Cohesive forces are what make a water droplet a drop. In other words, Cohesive forces are the intermolecular forces (such as those from hydrogen bonding and Van der Waals forces) which cause a tendency in liquids to resist separation. These attractive forces exist between molecules of the same substance. For instance, rain falls in droplets, rather than a fine mist, because water has strong cohesion which pulls its molecules tightly together, forming droplets. This force tends to unite molecules of a liquid, gathering them into relatively large clusters due to the molecules' dislike for its surrounding.
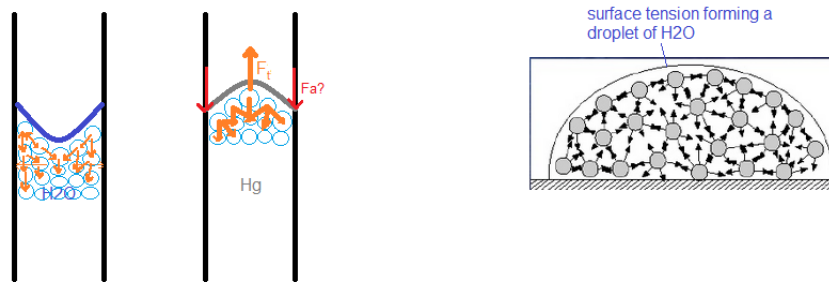

Figure 2.1.2: Test tube showing cohesive forces in a water drop[1]

As shown on Figure 2.1.2, cohesive forces gather the molecules together. For liquid water is confined in a tube, its surface (meniscus) has a concave shape because water wets the surface and creeps up the side.
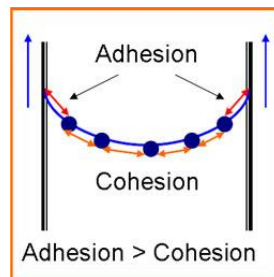

Figure 2.1.3: Test tube showing adhesive and cohesive forces between two substances[3]

Adhesive forces   Adhesive forces are the attractive forces between unlike molecules. They are caused by forces acting between two substances (figure 2.1.3), such as mechanical forces (sticking together) and electrostatic forces (attraction due to opposing charges). In the case of a liquid wetting agent, adhesion causes the liquid to cling to the surface on which it rests. When water is poured on clean glass, it tends to spread, forming a thin, uniform film over the glasses surface. This is because the adhesive forces between water and glass are strong

enough to pull the water molecules out of their spherical formation and hold them against the surface of the glass, thus avoiding the repulsion between like molecules.

Surface tension   To define the surface tension we use the apparatus shown in Figure 2.1.4. It consists of a C-shaped wire frame, on which is mounted a wire that can slide with negligible friction. The frame and sliding wire contain a thin film of liquid. Because surface tension causes the liquid surface to contract, a force F is needed to move the slider to the right and extend the surface. The surface tension is denoted by the Greek letter gamma (γ) and, as indicated by Equation 2.1.1 , is the magnitude F of the force per unit length L over which it acts.
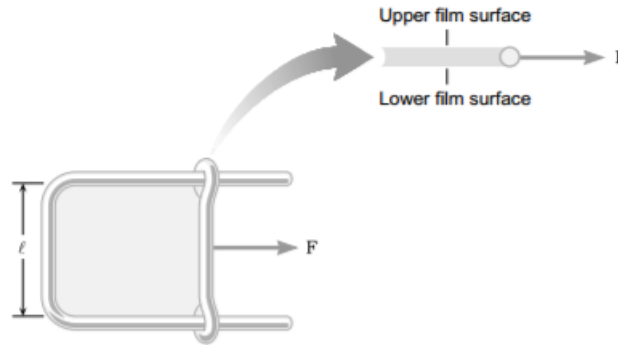

Figure 2.1.4: C-shaped wire frame and a wire slider[9]

The surface tension γ is the magnitude F of the force exerted parallel to the surface of a liquid divided by the length L of the line over which the force acts:

$$\gamma = \frac{F}{L} \tag{2.1.1}$$

SI Unit of γ : N/m

For the specific case illustrated in Figure 2.1.4, there is an upper surface and a lower surface, as the blow-up drawing indicates. Thus, the force F acts along a total length of $L = 2l$, where l is the length of the slider.

Pressure inside a Soap Bubble and a Liquid Drop   Anyone who's blown up a balloon has probably noticed that the air pressure inside the balloon is greater than on the outside. For instance, if the balloon is suddenly released, the greater inner pressure forces the air out, propelling the balloon much like a rocket. The reason for the greater pressure is that the tension in the stretched rubber tends to contract the balloon. To counteract this tendency, the balloon has a greater interior air pressure acting to expand the balloon.

A soap bubble has two spherical surfaces (inside and outside) with a thin layer of liquid in-between. Like a balloon, the pressure inside a soap bubble is greater than that on the outside. As we will see shortly, this difference in pressure depends on the surface tension γ of the liquid and the radius R of the bubble. For the sake of simplicity, let's assume that there is no pressure on the outside of the bubble ($P_o = 0$). Now, imagine that the stationary soap bubble is cut into two halves. Being at rest, each half has no acceleration and so is in equilibrium. According to Newton's second law of motion, a zero acceleration implies that the net force acting on each half must be zero ($\Sigma F = 0$). We will now use this equilibrium relation to obtain an expression relating the interior pressure to the surface tension and the radius of the bubble.
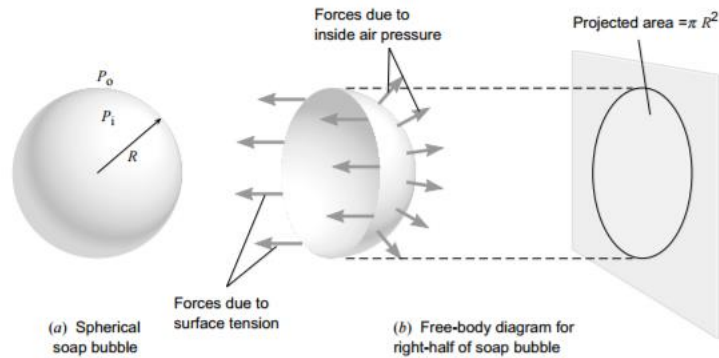

Figure 2.1.5: The inner and outer pressures on the spherical soap bubble are Pi and Po, respectively. The forces pointing to the left are due to the surface tension. The forces pointing perpendicular to the hemispherical surface are due to the air pressure inside the bubble.[9]

Figure 2.1.5 shows a free-body diagram for the right half of the bubble, on which two forces act. First, there is the force due to the surface tension in the film. This force is exerted on the right half of the bubble by the left half. The surface tension force points to the left and acts all along the circular edge of the hemispherical film. The magnitude of the force due to each surface of the film is the product of the surface tension γ and the circumference ($2\pi R$) of the circular edge, or $\gamma(2\pi R)$. The total force due to the inner and outer surfaces is twice this amount or $-2\gamma(2\pi R)$. We have included the minus sign to denote that this force points to the left in the drawing. We have also assumed the film to be sufficiently thin enough that its inner and outer radii are nearly the same. Second, there is a force caused by the air pressure inside the bubble. At each point on the surface of the bubble, the force due to the air pressure is perpendicular to the surface and is directed outward. Figure 2.1.5 shows this force at six points on the surface. When these forces are added to obtain the total force due to the air pressure, all the components cancel, except those pointing to the right. The total force due to all the components pointing to the right

is equal to theproduct of the pressure Pi inside the bubble times the circular cross-sectional area of the hemisphere, or $P_i(\pi R^2)$. Using these expressions for the forces due to the surface tension and air pressure, we can write Newton's second law of motion as:

$$\sum F = 0$$

$$\underbrace{-2\gamma(2\pi R)}_{1} + \underbrace{P_i(\pi R^2)}_{2} = 0 \qquad (2.1.2)$$

Part 1 is the force due to the surface tension.

Part 2 is the force due to the pressure inside the bubble.

Solving equation 2.1.2 for the pressure inside the bubble gives $P_i = 4\frac{\gamma}{R}$. In general, the pressure P_o outside the bubble is not zero. However, this result still gives the difference between the inside and outside pressures, so that we have:

$$P_i - P_o = \frac{4\gamma}{R} \qquad (2.1.3)$$

Spherical soap bubble

This result (equation 2.1.3) tells us that the difference in pressure depends on the surface tension γ and the radius R of the sphere. What is surprising is that a greater pressure exists inside a smaller soap bubble (smaller value of R) than inside a larger one.

A spherical drop of liquid, like a drop of water, has only one surface, rather than two surfaces, for there is no air within it. Thus, the force due to the surface tension is only one-half as large as that in a bubble. Consequently, the difference in pressure between the inside and outside of a liquid drop is one-half of that for a soap bubble:

$$P_i - P_o = \frac{2\gamma}{R} \qquad (2.1.4)$$

Spherical liquid bubble

Equation 2.1.4 is known as Laplace's law for a spherical liquid drop, after the French physicist and mathematician Marquis Pierre Simon deLaplace (1749–1827). This result also holds for a spherical bubble in a liquid, such as a gas bubble inside a glass of beer. However, the surface tension γ is that of the surrounding liquid in which the trapped bubble resides.

Part II

Work realised and Results

Chapter 3

Litterature review

3.1 Electric field :

Dr. ZimingWang wrote in an article[43] about methods describing the behavior of droplets under different circumstances of the electrical method of oily water separation. The results would be helpful to advance the design of the electro-coalescencers. Indeed, for a better understanding the researcher carried out numerous experiments both numerical and analytical to understand the behavior of the droplet deformation, breakup, coalescence and their dynamics under the influence of electric stress.

Three stages of the coalescence were described, that is to say the approximation of droplets , the process of film thinning/drainage, and film rupture leading to droplet–droplet coalescence. The article mentions the work of Rasin and Ristenpart in the approximation of droplets under strong electric fields and their behavior according to their size. But, the studies of droplets after coalescence are still minimized , which seems to be decisive in the coalescence of water droplets. Under certain conditions, the droplets can coalescence but breakup at last.

For a better understanding of the effect of the electrostatic on the coalescence of water droplets in oil, this articles presents 2 water drops into an insulating liquid. To produce the potential differences, a high-voltage power supply was used. The results of this experiments were discussed in details and throughout precise image processing.

Experimental details : The experiments were realized in a rectangular test cell made of Plexiglas (3 mm thickness) to facilitate visualization. The cell was 50(L) × 80(W) × 200(H) (mm3) in the internal dimensions and filled with white oil as an insulating liquid due to its dielectric properties and transparency. Two rectangular copper plate electrodes of 70 mm in width and 100 mm in length were placed parallel to the cell wall and were connected to a power supply. A D.C. high voltage power supply was used to generate electric potential

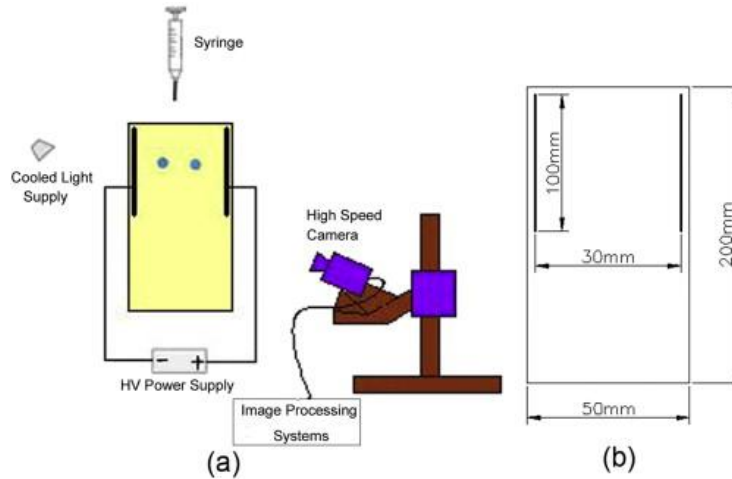differences between the electrodes. (Figure 3.1.1)

Figure 3.1.1: Schema of the apparatus

Many results were noted such as density, viscosity, the interfacial tension and conductivity of the water droplets.

Results : The calculation of the different parameters were made thanks to several equations, and the effect of each case was supported by detailed image processing.

- The drops approach in a higher velocity when they become closer to each other. And the velocity becomes higher under stronger field strength.

- The velocity of droplets moving towards each other in electric field is higher than that in gravity field. If the collisional kinetic energy is sufficient to expel the intervening film between the two droplets, coalescence will occur. So, the electric field favorite the drops to coalesce instantly or temperately.

- Above the critical field strength of about 200 kV/m, the drops fail to coalesce.

- Higher electric field strength generates longer **time to coalesce**[1] and restore.

- The **bridge**[2] radius is an important factor that reflects the coalescence process.

- The pressure of the bridge is lower than that of the droplets if the strength of electric is lower than Ec (Electical field).

---

[1]The period in which the bridge between the droplets becomes cylinder from contact.
[2]Space between the equators of the two drops.

- These experiments revealed that the electric force can facilitate drops to coalesce, by enhancing the drops to be collision with each other. But a higher electric force would induce the drops to be separated after contact.

3.2   Electrohydrodynamics field

Aggregation and coalescence of oil droplets in water via electrohydrodynamic flows

In this article[28], the scientists proved that electrohydrodynamic flows induce immiscible oil droplets to coalesce. They found that the best way to make the droplets coalescing is to suddenly decrease the applied frequency.

Numerical simulation of the electrohydrodynamic effects on bubble rising using the SPH method

The method utilized in this paper[32] is the Lagrangian Incompressible Smoothed Particle Hydrodynamics (ISPH). An electric field is applied on a bubble under different values of Reynolds, Bond and electrical Capillary Number (effect of viscous forces versus surface tension acting across the interface of the two liquids). The bubble elongates in the direction of the electric field forming a prolate shape. If the electric field is applied on two bubbles which are placed on a vertically line, they tend to coalesce due tout the prolate deformation.

A phase field numerical study of 3D bubble rising in viscous fluids under an electric field.

In this article[30], they use an electric-fluid-flow model to simulate the evolution of electric field and the deformation of rising bubble. Therefore, they resolved Laplace equation, Navier Stokes equation and Cahn-Hilliard equation. The vertical electric fluid increases the velocity of the ascending of the bubble whereas a horizontal electric field decreases it.

Numerical and experimental study on electric field driven coalescence of binary falling droplets in oil

They developed in this paper[34] a model based on Computational Fluid Dynamics technique and an electrostatic model. They found that electrocoalescence rate could be improved by using a stronger electric field or closer drops.

Numerical Simulation of bubble dynamics in a uniform electric field by the adaptative 3D-VOSET method

In this paper[31], the authors used a model which couples the Navier Stokes equation and electric field equation. Increasing the electric Bond number or the ratio of electrical permittivity enable a larger deformation and rises the velocity of the bubble.

A smoothed particle hydrodynamics study on the electrohydrodynamic deformation of a droplet suspended in a neutrally buoyant Newtonian fluid

In this paper[29], they simulated a 2D Lagrangian two phases numerical model and they studied the deformation of a drop subjected to the effects of viscous, surface tension and electric forces. Using the Smoothed Particle Hydrodynamics method, they proved that imposing constant electrical potentials

to upper and lower horizontal boundaries results in a deformation of the drop to a prolate or oblate shape.

The effect of normal electric field on the evolution of immiscible Rayleigh-Taylor instability

In this paper[33], scientists studied the forces acting at the interface of two fluids using a Smoothed Particle Hydrodynamics method by varying electric permittivity and conductivity ratio and electric field intensity. They observed that increasing top-to-bottom permittivity ratio increases the rising velocity of the bubble whereas increasing top-to-bottom conductivity ratio has the opposite result. These results are amplified at larger electric field intensities.

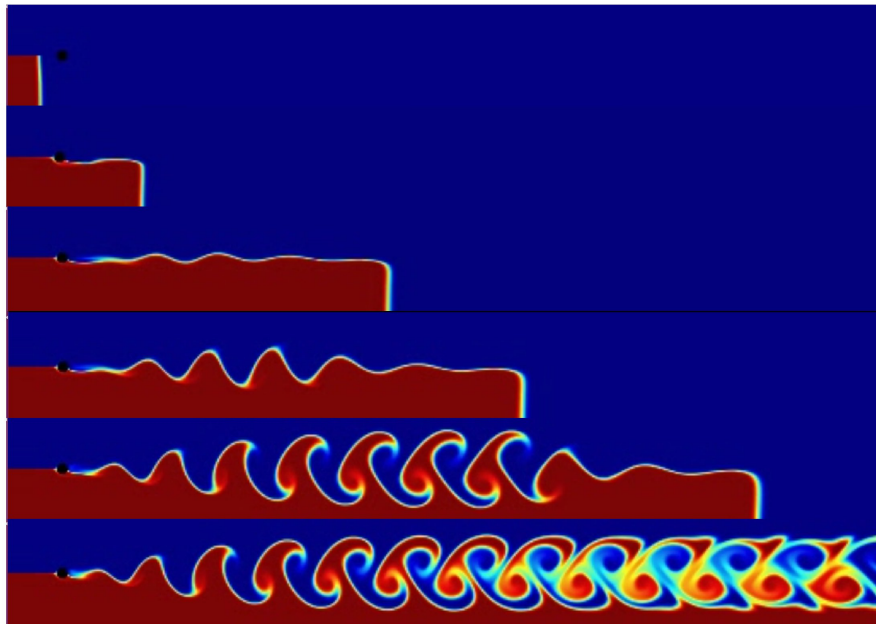# Chapter 4

Simulations

4.1   Cylinder

Figure 4.1.1: Simulation of a bubble in a cylinder

An example of 2D viscous flow around a simple solid boundary. Fluid is injected to the left of a channel bounded by solid walls with a slip boundary condition. A passive tracer is injected in the bottom half of the inlet. Adaptive refinement is used based on both the vorticity and the gradient of the passive tracer (Figure

4.1.1). After an initial growth phase, a classical Bénard–von Kárman vortex street is formed.
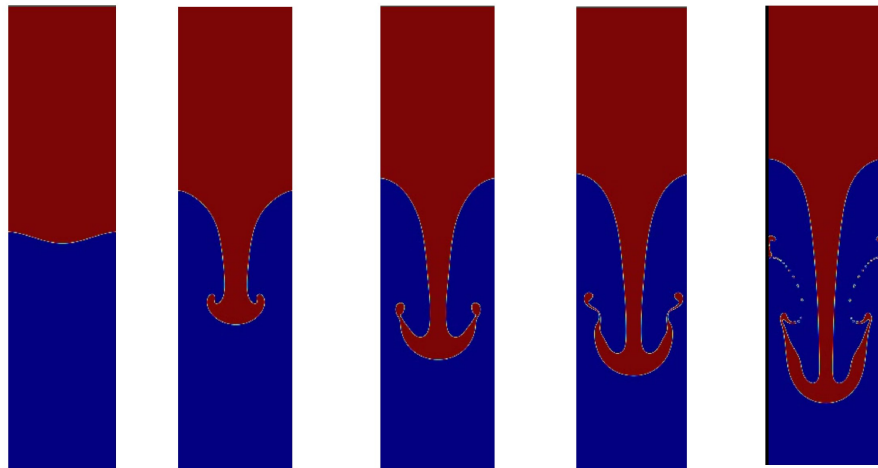
4.2   Rayleigh-Taylor instability

Figure 4.2.1: Simulation with the RTL model

A classical test case for the flow of two fluids of different densities. A sinusoidal interface separates the two fluids. The heavier fluid is on top. As shown on Figure 4.2.1, a mushroom-shaped instability develops in time.

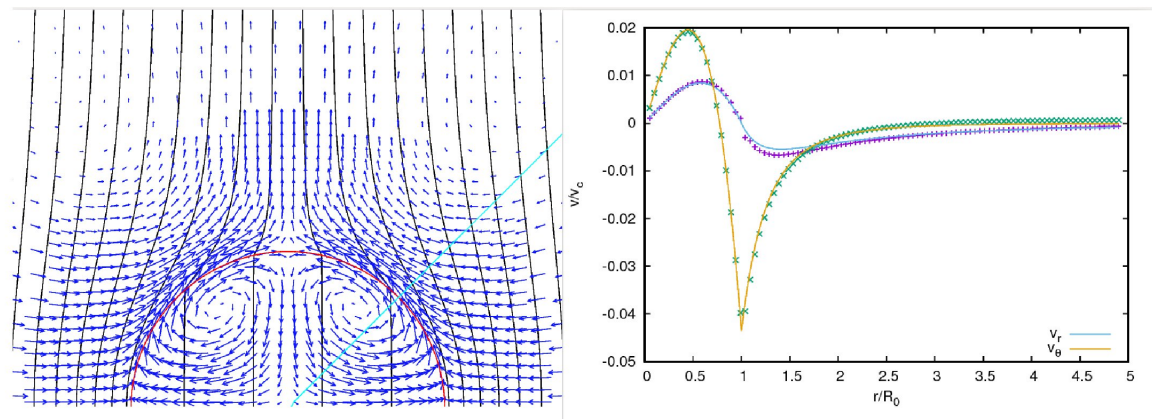## 4.3 Equilibrium of a droplet suspended in an electric field

Figure 4.3.1: Simulation of a drop suspended in an electric field

A conducting droplet is suspended in a conducting liquid of the same density. A constant horizontal potential difference is imposed far from the droplet. At equilibrium, surface tension balances the normal electrical stresses while recirculations are induced by tangential electrical stresses due to the variable charge distribution along the interface.

Figure 4.3.1 left : Axisymmetric numerical solution in stationary regime. Equipotential lines (black), interface (red), velocity field (blue) and 45 degrees transect line (light blue).

Figure 4.3.1 right : Radial and azimuthal components of the velocity along a 45 degrees transect.
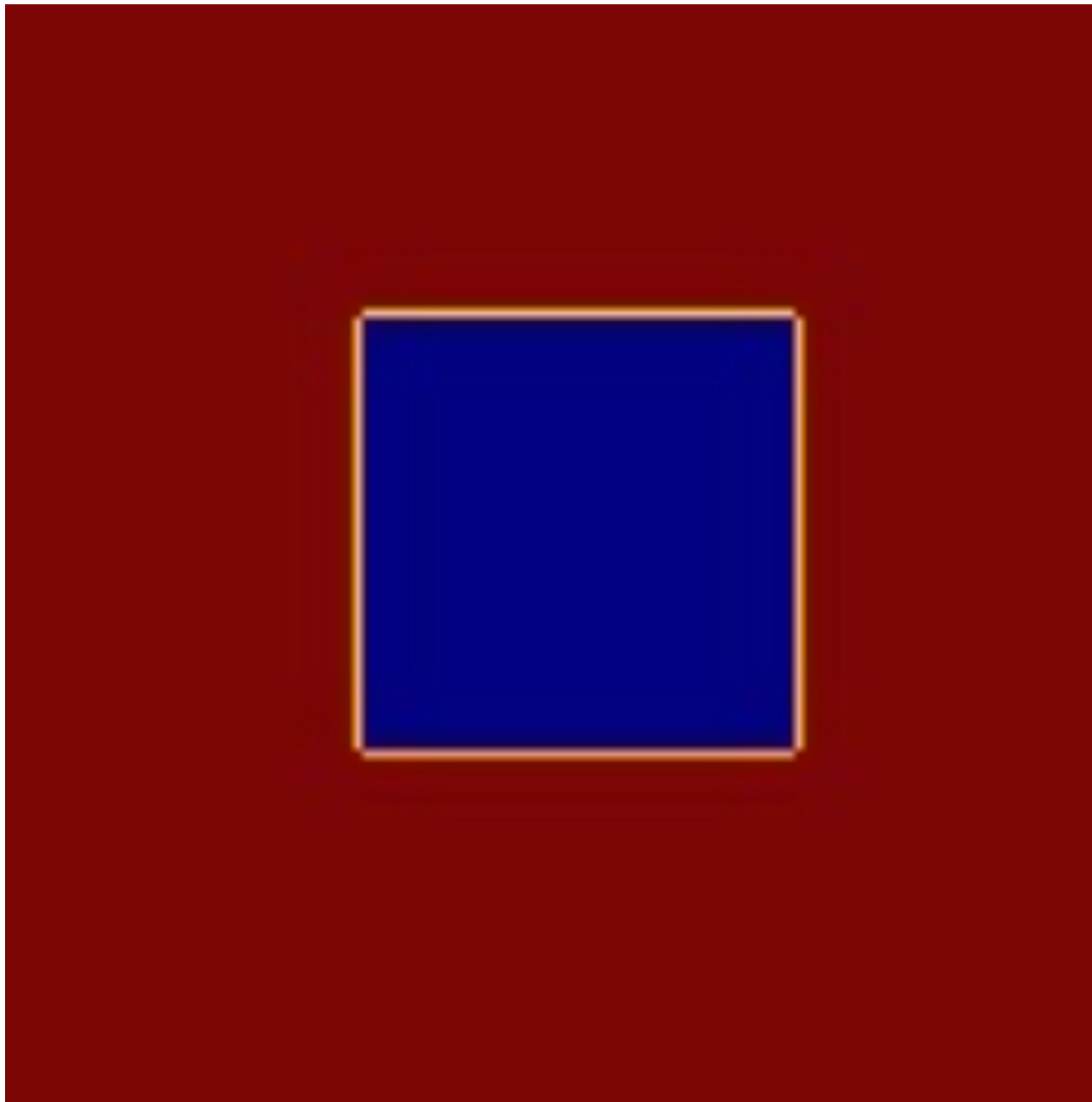
4.4   Squared bubble

Figure 4.4.1: Squared bubble

When simulating the bubble rising effect with a square bubble in a fluid by ignoring the gravity effect, the squared bubble becomes circular due to the surface tension. The fluid inside the bubble tend to decrease its interface with the other fluid. This result is shown by Figure 4.4.3. During the simulation, the bubble rises a little.

Conclusion

Thanks to this project, we have learned about the methods used in the water/oil separation in the petroleum industries. We were able to understand the physics and the mathematical elements, such as Laplace's Law, the Navier-Stokes equations, the surface tension, that are behind this important notion. It also enabled us to learn more about the effects of each parameter on the feasibility of each method.

One of difficulties we encountered during this project was the fact that it was entirely written and made in english, but this helped us learn to carry out research in english, and overcome some of our struggle with scientific terms. We discovered new ways of finding articles corresponding to our research, using bibliographies and particular sites that are offered by our school. Eventhough we had a few coordination problems due to the different schedules of each member of the group, we managed to find a regular pace of work, which helped us in our research but also in our report. Last but not least, we had to learn a totally new programming language for us which is Gerris. At first we struggled a bit to understand the syntax, but thanks to our professor's directions and the Gerris forum users' help, we became more familiar with the software and were even able to write our own program and run a simulation based on it.

Annex

A/ Techniques

Gravity separation

The separators in the oil industry are gravity separators vessels. They have some particularities and things on common. Obviously, they all rely on gravity force to achieve separation. The gravity separator vessels perform at high efficiency and the separation is enhanced in the gravity section by internals that ensures good flow distribution. Plus, while dimensions of the separator are minimized, enhanced gravity separation of oil and water results in a maximum overall performance of the separator.

1 Trash trap (inclined rods)
2 Oil retention baffles
3 Flow distributors (vertical rods)
4 Oil layer
5 Slotted pipe skimmer
6 Adjustable overflow weir
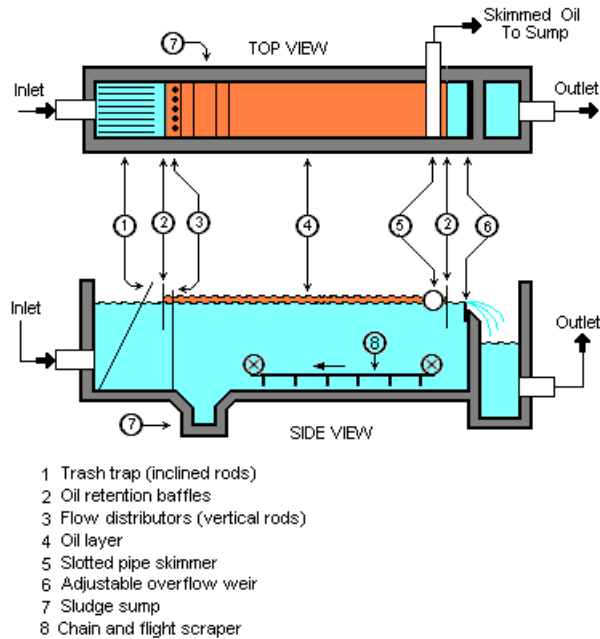7 Sludge sump
8 Chain and flight scraper

Figure 4.4.4: Schema of a typical gravimetric API separator.

For example the API separator (Figure4.4.4) is a gravity separation device [10]. It define the rise velocity of oil droplets based on their density, size and water properties (Using Stokes law principles). In fact it's a device designed to separate gross amount of oil from all oily water sources (chemical plants, petrochemicals plants, oil refineries..). It is named like that because a lot of separators are based on standards published by the American Petroleum Institute. The design of the device is based on gravity difference between oil and wastewater (much smaller than the specific gravity difference between suspended solids an water). While the suspended solids are attracted in the bottom of the separator, the oil will rise to top and the the wastewater will be in the middle between oil and solids.

Figure 4.4.5: Different plate separators

Plate separators, or Coalescing Plate Separators (Figure 4.4.5)[21] are similar to API separators ; they are also based on Stokes Law principles, but include inclined plate assemblies (parallel packs)[20]. Gravitation separation of oil and water is accomplished by droplet settling. It requires such a long time and this is why a plate pack coalescer is used in the liquid section to maximize the degree of liquid-liquid separation. This principle of parallel plate separators relies on the density difference between the oil and water phase.

Filtration

After decantation or centrifugation, the solid and liquid bodies are separated (in the same vessel). The filtration allows the physically separation of the solid from a liquid by passing the mixture through a filter more or less big. The solid bodies (called residues) are trapped in the filter and the liquid (filtrate) is recovered in a container.

In the case of the petroleum industry, filtration requires advanced processes. However, the water produced by the petroleum industry has always been considered a waste even if it can be reused. But nowadays the industries proceeed to water treatment through the filtration process. To begin with, the injection of a coagulant allows the coagulation of solid particles and oil. The coagulated particles are then separated from the water using a water / oil separation system. The finer particles can be removed by multimedia filtration or by ultrafiltration. In water treatment, multimedia filtration refers to a mixture of sand, gravel and anthracite that eliminates both dirt and solids. The effluent passes through a sand filter where the bacteria has previously been developed. Ultrafiltration is a technique for separating the elements contained in a liquid. It uses semi-permeable membranes whose pore diameter is between 0.001 and 0.1 micrometer. However this keeps the water not completely cleaned, some pollutants persist such as dissolved ions. Desalination technologies can be used

(nanofiltration, ion exchange, etc.) to separate these pollutants from water. Some petroleum industries achieve 80-90% water that can be reused or disposed of safely
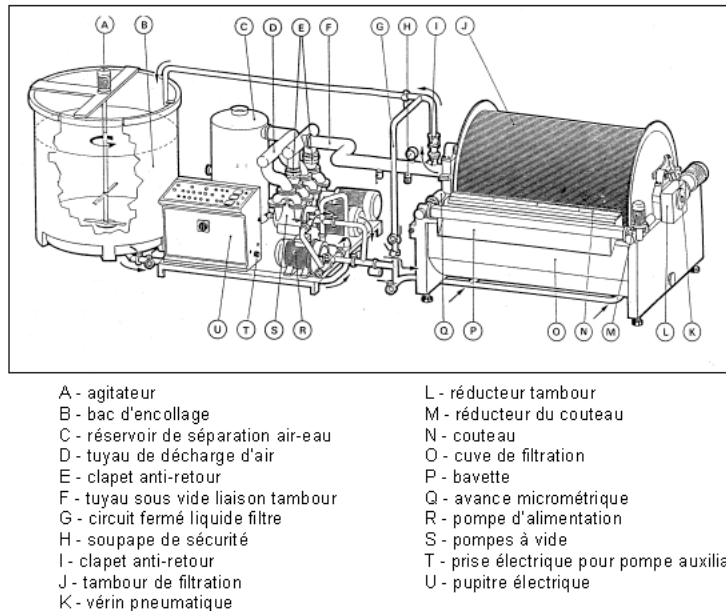

A - agitateur
B - bac d'encollage
C - réservoir de séparation air-eau
D - tuyau de décharge d'air
E - clapet anti-retour
F - tuyau sous vide liaison tambour
G - circuit fermé liquide filtre
H - soupape de sécurité
I - clapet anti-retour
J - tambour de filtration
K - vérin pneumatique

L - réducteur tambour
M - réducteur du couteau
N - couteau
O - cuve de filtration
P - bavette
Q - avance micrométrique
R - pompe d'alimentation
S - pompes à vide
T - prise électrique pour pompe auxiliaire
U - pupitre électrique

Figure 4.4.6: Explained schema of a vacuum filter

Vacuum filtration The most widely used vacuum filters(Figure 4.4.6) are of the open drum type. The rotary drum filter essentially consists of a rotating drum partially immersed in a tray containing the sludge to be filtered. This drum is formed by several sealed compartments covered with a cloth serving as a filtration support. Adding a precoat is the only possibility of filtration in the case of refinery sludge.

[22, 2, 36]

Chemical separation

The main method used in the fuel-industry to separate oil from water is called demulsification. Oil demulsification can defined as the breaking of a crude oil **emulsion** into oil and water phases (Emulsion being a mixture of two or more immiscible liquids, here the oil is called the dispersed phase and water the dispersion medium). The Figure 4.4.7, shows a water in oil emulsion.

In the industrial point of view, three aspects are essential in the use of the method:

- The rate or the speed at which this separation takes place

- The amount of water left in the crude oil after separation
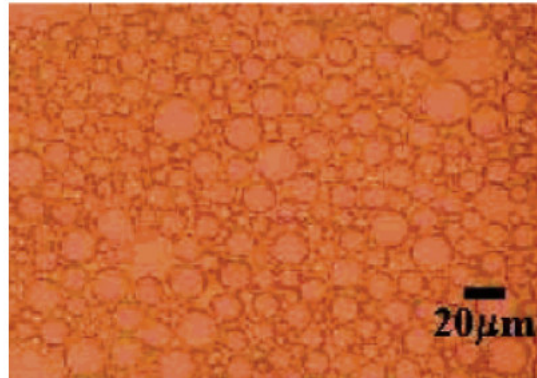- The quality of separated water for disposal

Figure 4.4.7: Picture of a water in oil emulsion

Mechanism :   Among all methods used in the demulsification process we can find the chemical methods. The most common method of emulsion treatment is adding demulsifiers. These chemicals are designed to neutralize the stabilizing effect of emulsifying agents. Demulsifiers are surface-active compounds that, when added to the emulsion, migrate to the oil/water interface, rupture or weaken the rigid film, and enhance water droplet **coalescence**.

Demulsifiers usually contain three components:

- Solvents such as benzene, toluene, xylene, short-chain alcohols, and heavy aromatic naphtha,

- Surface-active ingredients which are chemicals that have surface-active properties characterized by hydrophilic-lipophilic balance (HLB) values.

- Flocculants which is a substance added to a suspension to enhance aggregation of the suspended particles.
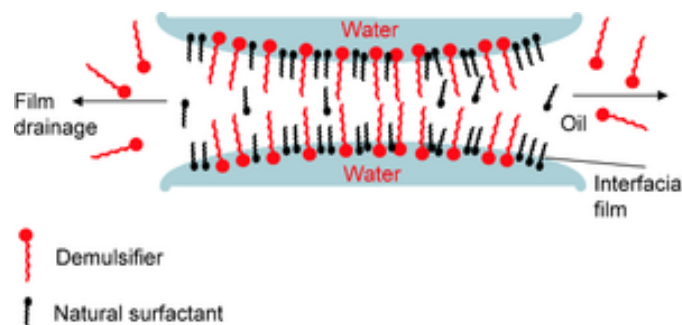

Figure 4.4.8: Schema of the film drainage process

Figure4.4.8 shows the film drainage process schematically. When two droplets approach each other, the thickness of the interfacial film decreases as the liquid flows out of the film. This sets up an Interfacial Tension (IFT) gradient with high IFT inside the film and low IFT outside the film. The interfacial viscosity is very high because of the adsorbed natural surfactants (asphaltenes). Demulsifier molecules have a higher surface activity than natural surfactants and, therefore, replace them at the interface. When demulsifier molecules are adsorbed in the spaces left by the natural surfactants, the IFT gradient is reversed, film drainage is enhanced, and the interfacial viscosity is reduced. This causes the film to become very thin and collapse, resulting in droplet coalescence. The efficiency of the demulsifier thus depends on its adsorption at the droplet surface. There is competition for adsorption when other surface-active species are present. The indigenous surfactants, like asphaltenes, present in the crude oil are only weakly adsorbed and are readily displaced by the demulsifier.

Optimum emulsion breaking with a demulsifier requires a properly selected chemical for the given emulsion; adequate quantity of this chemical; adequate mixing of the chemical in the emulsion; and sufficient retention time in separators to settle water droplets. As stated before, for any given emulsion, the selection of the right chemical as a demulsifier is crucial to emulsion breaking. When the right demulsifier has been chosen, there remains another crucial part which is the dosage of this chemical. As a matter of fact, many factors affect demulsifier performance including temperature, type of crude oil, droplet size and distribution and pH.

Advantages and disadvantages: This process is effective and fast-acting. However, it is a complex method because it is necessary to find the appropriate demulsifier according to the type of crude oil and others conditions such as temperature. Each type of crude oil requires a specific demulsifier. Moreover, some problems can be encountered by the removal of the demulsifiers into the water or the oil. Finally, this method is costly because it requires equipment for mixing or agitation and chemical products.

[6, 17, ?]

pH adjustment separation

As said previously, the pH affects the demulsifier performance. Generally, basic pH promotes oil-in-water emulsions and acidic pH produces water-in-oil emulsions. High pH, therefore, helps in destabilizing water-in-oil emulsions. It is also known that basic pH reduces demulsifier dosage requirements.

The following graph (Figure 4.4.9) shows how the performance of different 30 ppm (parts-per million) demulsifiers depending on their pH and for how long they have been used. We can see that for an optimal duration of demulsifier use (one hour), demulsifiers with basic pH (10) have the highest percentage of water separation.
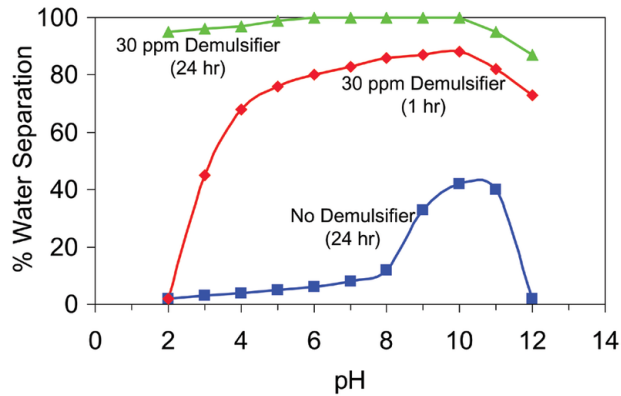
[7, 23]

Figure 4.4.9: Graph showing the performance of different demulsifiers

Heating treatment

The process of heating treatment consists in transforming water into steam by heating up the oil to 200°C. Moreover, the heating process reduces the oil viscosity and then facilitate the escape of water steam produced. Heating increases molecular movement which enhances the coalescence of water droplets. It might accelerate the demulsifiers action. It also might increase the gravity difference between oil and water to enhance the gravimetric separation.

Advantages/Disadvantages: Heating accelerates emulsion breaking. A part of oil is also vaporised. It can be condensed later in the process with the gas. But it still causes a loss of volume. When crude oil is heated, some gas is liberated and causes a problem of treatment and requires appropriated equipment. This process is costly because of the fuel required for the heating and the treatment of the gas liberated. [4]

Membrane filtration

Membrane technology has become a significant separation technology over the past decennia. The applications of membrane technology have spread and become an essential separation technology. The advantages of membrane technology are that it works without addition of chemicals, with lower energy requirement, is easy to handle and has well-arranged process conductions. Membrane separation already shows more efficiency as compared to conventional techniques and efficiency depends entirely on the membrane itself. As shown on Figure 4.4.10, the separation is very simple: the membrane acts as a semi-permeable layer between two phases and it regulates the transportation between those two phases. Specifically, the filter will let water flow through the membrane, while it catches suspended solids and other substances.
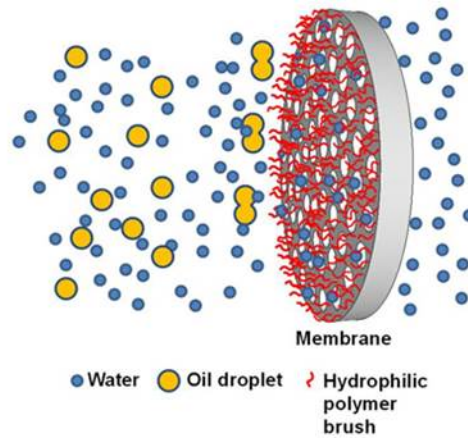
Figure 1: Filtration of an oil-water mixture with a membrane coated by a polymer brush. The brush will help reduce membrane fouling.

Figure 4.4.10: Schema of the process of membrane separation

Membrane separation processes have increasingly become a viable alternative method for oil–water separation. The chart (Figure4.4.11) shows the schematic representation of the basic principle involved in the membrane separation. [24, 8, 19]
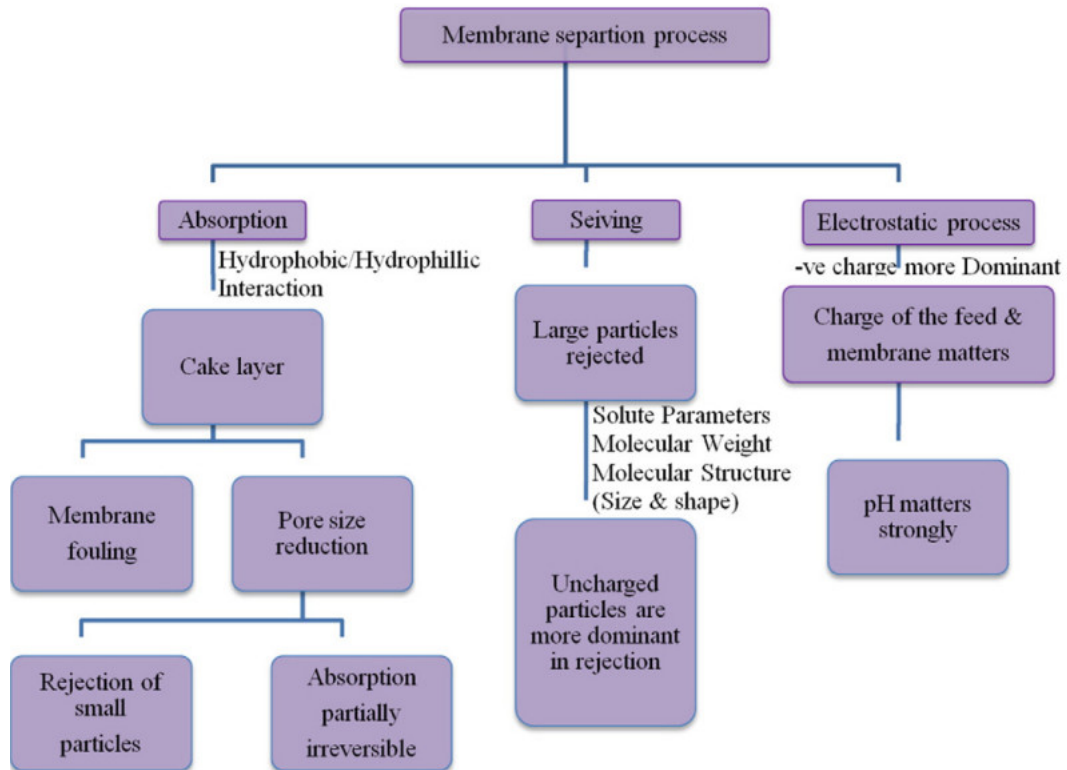
Figure 4.4.11: Diagram explaining the membrane separation process

Centrifugal separation

This technique separate oil and water by centrifugation. Centrifugation means, according to Wikipedia, a process which involves the application of the centrifugal force for the sedimentation of heterogeneous mixtures with a centrifuge, and is used in industrial and laboratory settings. It is made of stainless steel (on the inside), brass and bronze and is designed to separate two miscible or partially miscible substances.

Mechanism: As shown on Figure 4.4.12[25], the design of this device includes generally a moving cylindrical container inside a lager one which is stationary. The mixed oil-water liquid is pumped with a constant speed, at a certain angle in the apparatus, which creates a spinning **vortex**[1]. As a result from the rotation, the denser liquid which is water move to the outside and the lower-denser one
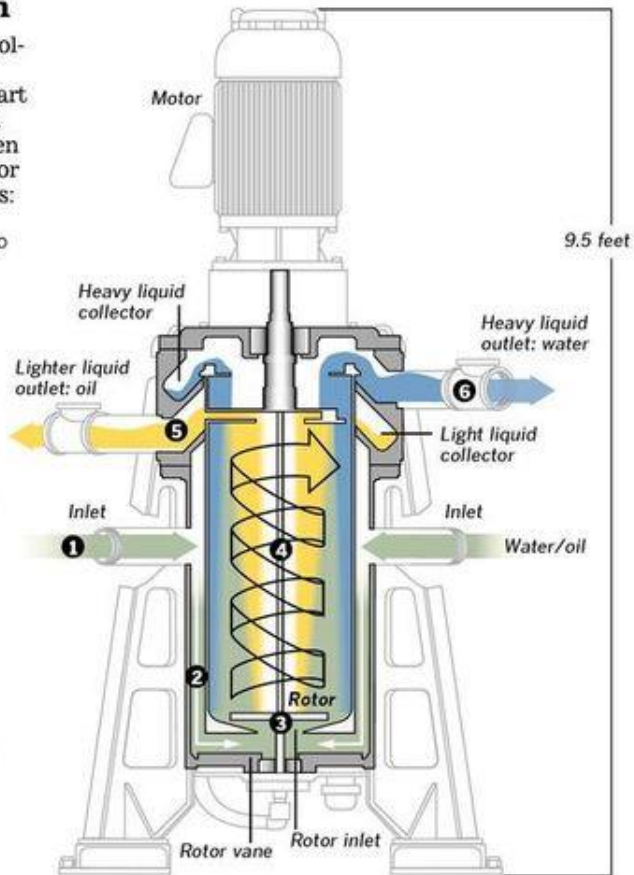
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[1]A vortex is a region in a fluid in which the flow rotates around an axis line, which may be straight or curved

stays in the center of rotation and is collected at the end of the filtration.

Spinning solution

Centrifugal separator technology owned by actor Kevin Costner could prove to be part of the solution to the gulf oil spill. Costner's team has been working on the technology for about 15 years. How it works:

❶ **Water/oil** mix can flow into either or both of two inlets

❷ It is **pumped or flows** via gravity to the bottom of the separator.

❸ **Rotor vanes** direct the oil and water into the **rotor**.

❹ **Spinning rotor** generates centrifugal force up to 600 times the force of gravity. As mix rises, the lighter-density oil flows toward the center of the rotor; the heavier water is forced outward.

❺ Liquids move into separate **collectors**

❻ **Oil and water** leave the separator through different **outlets** to either be collected in a tank (oil) or returned to the sea (water).

Motor

9.5 feet

Heavy liquid collector

Heavy liquid outlet: water

Lighter liquid outlet: oil

Light liquid collector

Inlet

Inlet

Water/oil

Rotor

Rotor vane

Rotor inlet

Source: CINC Industries. Graphics reporting by TOM REINKEN

MARK HAFER Los Angeles Times

Figure 4.4.12: Schema explaining centrifugal separation process

Advantages and disadvantages : The centrifugal separator is more efficient than other devices using gravitational forces. While the spinning **vortex** is created by pumping the oily water, it creates a powerful force that separate these two components. Unlike the gravitational separators, this device's force is approximately 1000 times more important. However, they have some drawbacks and namely the low powered suction problem. Indeed, they are not powerful enough to lift the mixture into the separator. So it has to be primed before use. [11, 18]

B/Maxwell Equations

Maxwell's or Maxwell-Lorentz's equations are fundamental laws of physics. They define the postulates of electromagnetism, with the electromagnetic force of Lorentz. Maxwell's equations had different local forms (as we have seen in the course of electromagnetism) such as the Gaussian, Ampère or Faraday theorem until Maxwell assembled them in the form of equations integrals. The latter prove that the electric and magnetic fields are independent of one another while they are not in variable regime. We are talking about an electromagnetic field.

Maxwell's equations are four (Maxwell-Gauss, Maxwell-Faraday, Maxwell-Thomson and Maxwell Ampère). All these equations relate to electromagnetism and the description of several magnetic, electrical and luminous phenomena.

Maxwell's equations are four (Maxwell-Gauss, Maxwell-Faraday, Maxwell-Thomson and Maxwell Ampère). All these equations relate to electromagnetism and the description of several magnetic, electrical and luminous phenomena.

Maxwell-Gauss

This formula stipulates that the divergence of the electric field is proportional to the distribution of electrical charges. (E is the electric field in V / m, q the charge distribution and εo the dielectric permittivity of the vacuum).

$$div(\overrightarrow{E}) = \frac{\rho}{\varepsilon_0} \tag{4.4.1}$$


E
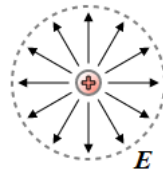
This equation means that the electric field is divergent (or converge according to the sign of the load) from a source (positive charge on the diagram). Div E is therefore proportional to the distribution of charges.

Maxwell-Thompson

The Maxwell-Thompson formula (or Maxwell-Flux) explains that the divergence of the magnetic field is zero. The lines of magnetic field come out of a positive (or negative) pole to go in the opposite direction, they do not diverge. It is therefore concluded that there is no magnetic monopole north or south because all the magnets have 2 poles.
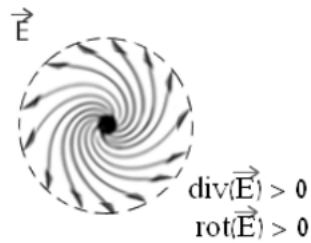
$$div(\overrightarrow{B}) = 0 \qquad (4.4.2)$$
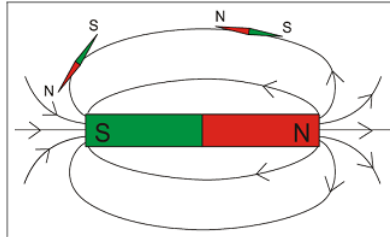
Maxwell-Faraday

The Maxwell-Faraday formula is the induction phenomenon and explains that the rotation of the electric field E is inversely proportional to the variation of the magnetic field over time. It is this variation of magnetic field over time that produces an electric field and not the magnetic field alone.
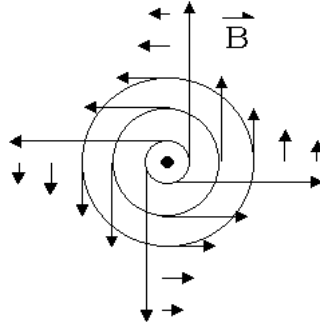
$$\overrightarrow{rot}(\overrightarrow{E}) = -\frac{\partial \overrightarrow{B}}{\partial t} \qquad (4.4.3)$$

$$\text{div}(\overrightarrow{E}) > 0$$
$$\text{rot}(\overrightarrow{E}) > 0$$

Maxwell-Ampere:

The Maxwell-Ampere formula states that the magnetic field rotational depends on a variation of the electric field over time (dE / dt) and also depends on an electric current (μ0 × j).

$$\overrightarrow{rot}(\overrightarrow{B}) = \mu_0 \overrightarrow{J} + \frac{1}{c^2}\frac{\partial \overrightarrow{E}}{\partial t} \qquad (4.4.4)$$

The vector B is the magnetic field, the constant μ0 is the magnetic permeability in the vacuum, j is the current density vector and c is the celerity of light (constant).

[14, 26, 16]

C/ Equation of static fluid at rest

Fundamental equation of static fluids at rest

This paragraph comes from the "Fundamentals of Fluid Mechanics" , Munson.[41]
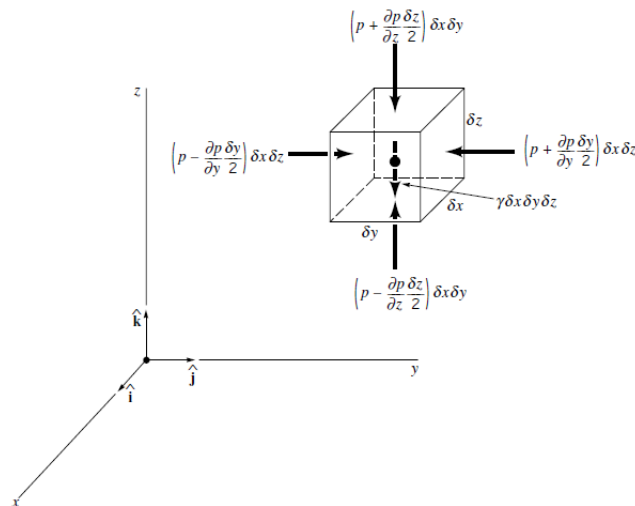

Figure 4.4.13: Forces applied on a small square or fluid

We consider a small rectangular element of fluid on which two forces are acting : surface forces due to pressure and body forces which are the weight. On the Figure 4.4.13, pressure forces are represented acting on every sides of

the box. The pressure of the center is designated by p, therefore the pressure on the faces is expressed in terms of p and derivatives.

Expression on the surface forces : The resultant force in z direction is :

$$\delta F_{\mathrm{Z}} = (p - \frac{\partial p}{\partial z}\frac{\delta z}{2})\delta x\delta y - (p + \frac{\partial p}{\partial z}\frac{\delta z}{2})\delta x\delta y \tag{4.4.5}$$

$$\delta F_z = -\frac{\partial p}{\partial z}\delta x\delta y\delta z \tag{4.4.6}$$

In the same way, the resultants forces in x and y directions are :

$$\delta F_x = -\frac{\partial p}{\partial x}\delta x\delta y\delta z \tag{4.4.7}$$

$$\delta F_y = -\frac{\partial p}{\partial y}\delta x\delta y\delta z \tag{4.4.8}$$

The resultant surface force can be expressed as :

$$\delta\overrightarrow{F_s} = \delta F_x\,\overrightarrow{i} + \delta F_y\,\overrightarrow{j} + \delta F_z\,\overrightarrow{k} \tag{4.4.9}$$

The pressure gradient is :

$$\nabla p = \frac{\partial p}{\partial x}\overrightarrow{i} + \frac{\partial p}{\partial y}\overrightarrow{j} + \frac{\partial p}{\partial z}\overrightarrow{k} \tag{4.4.10}$$

Then by combining the 3 equations 4.4.7,4.4.8 and 4.4.6:

$$\delta\overrightarrow{F_s} = -\nabla p\delta x\delta y\delta z \tag{4.4.11}$$

Expression of body forces : The force of the weight $\delta\overrightarrow{F_B}$ is on the vertical axis z :

$$-\delta F_B\,\overrightarrow{k} = -g\delta m\,\overrightarrow{k} \tag{4.4.12}$$

In cartesian coordinates :

$$\delta m = \rho\delta V = q\rho\delta x\delta y\delta z \tag{4.4.13}$$

With equation 4.4.13, equation 4.4.12 becomes :

$$-\delta F_B\,\overrightarrow{k} = -\rho g\delta x\delta y\delta z\,\overrightarrow{k} \tag{4.4.14}$$

Expression of global force :

$$\delta\overrightarrow{F} = \delta\overrightarrow{F_s} + \delta\overrightarrow{F_B} \tag{4.4.15}$$

$$\delta\overrightarrow{F} = -(\nabla p + \rho g\,\overrightarrow{k})\delta x\delta y\delta z \tag{4.4.16}$$

The Newton's second law applied to a fluid rest ($\overrightarrow{a} = \overrightarrow{0}$) can be expressed as :

$$\sum \delta\overrightarrow{F} = \delta m\,\overrightarrow{a} = \rho\delta x\delta y\delta z\,\overrightarrow{a} = \overrightarrow{0} \tag{4.4.17}$$

The final equation is :

$$\delta\overrightarrow{F} = \overrightarrow{0} \implies \nabla p + \rho\,\overrightarrow{g} = \overrightarrow{0} \tag{4.4.18}$$

In component forms :
$-\frac{\partial p}{\partial x} + \rho g_x = 0$ or $g_x = 0$ so $\frac{\partial p}{\partial x} = 0$
$-\frac{\partial p}{\partial y} + \rho g_y = 0$ or $g_y = 0$ so $\frac{\partial p}{\partial y} = 0$
$-\frac{\partial p}{\partial z} + \rho g_z = 0$ or $g_z = -g$ so $\frac{\partial p}{\partial x} = -\rho g = -\gamma$ where γ is the specific weight of the fluid.

The fundamental equation for fluids at rest is :

$$\frac{dp}{dz} = -\gamma \tag{4.4.19}$$

Equation 4.4.19 shows that the pressure depends only on the z component.

Navier-Stokes equation

For an incompressible fluid :

$$\frac{\partial u}{\partial t} + (u\cdot\nabla)u = -\frac{\nabla p}{\rho} + \nu\nabla^2 u + f \tag{4.4.20}$$

u is the velocity of the fluid parcel
p is the pressure
ρ is the fluid density
ν is the kinematic viscosity
f is the external source

D/ Litterature review

Chemical treatment

The chemical treatment consists in adding demulsifiers to the emulsion in order to enhance the coalescence of the water droplets and then separate them from the oil. The demulsifiers are chosen according to many parameters such as the temperature, the droplets dimension or the type of oil.

Type of oil

Some scientists have studied in a paper[**?**] the effects of different demulsifiers on medium crude oil and heavy crude oil. They studied the existing demulsifiers and proposed a new formulation for the demulsification of heavy crude oil emulsion. They carried out many tests on bottle tests. First, they tested demulsifier from water soluble and oil soluble groups by fixing the concentration of the surfactant and the temperature. Then, they chose the best surfactant of the two groups and made tests by varying the concentration of the surfactant. Finally, they combined three surfactants and compared its effectiveness with other commercial demulsifiers.

The results of each tests are shown by graphics where the separated volume fraction is plotted versus the time. As a result, we see the three steps of the process. First, the droplets come nearer. Then, the surfactant drains the thin film of the drops. Finally, the thin film breaks and the drops coalesce. The first step depends on physical parameters. The formulation of the surfactant takes action only in the second step.

They did tests with stable emulsions. They mixed water containing surfactants with the two types of oils, at 70°C. The emulsions prepared contained 20% of water. Then, they transferred the emulsions in graduated bottle tests, shook them and recorded the position of the oil/water interface every 5 minutes.

They have found that the best surfactants for the medium oil were not efficient as well for the heavy crude oil. They said that it might be due to the lower asphaltene 3 content of medium crude oil relative to heavy crude oil. In heavy crude oil, single demulsifiers have low efficiency. Moreover, they proved that demulsifiers with moderate water solubility and low oil solubility are well efficient. They also proved that the reduction of the interfacial tension is a significant parameter and that the water separation rate is proportional to the reduction of interfacial tension.
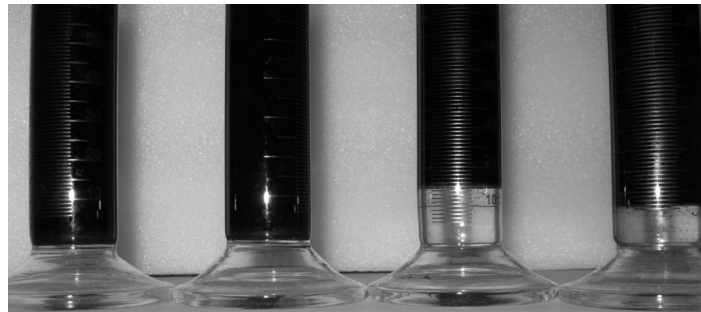

Figure 4.4.14: Bottle testing results for choosing the best composite of single chemical demulsifiers for the demulsification of heavy crude oil.

On the Figure 4.4.14, the two first bottles from the left are heavy crude oil whithout any surfactants, the third bottle contains the new formulation of

demulsifier, and the last one contains a commercial formulation, the V-4654, a blend of surfactants, cosurfactants, wetting agents, flocculating agents and coalescers. As shown on the figure, the new formulation is better than the commercial formulation. The final formulation is a mixture of phenolic resins (alkoxylated alkyl phenol formaldehyde resin NPFE), a surfactant named EO/PO block copolymer (ethylene oxyde/propylene oxyde) and the methyl trioctyl azanium chloride (TOMAC). Those surfactants have been chosen beacause of their low interfacial tensions.

Type of surfactant	Cationic	Anionic	Nonionic	Zeitterionic
Advantages	- Form stable solutions in brine - Cationic surfactants or mixtures of them with nonionic surfactants are the most effective EOR agent for carbonate reservoirs	- Effective candidate for sandstone reservoir	- Effective for surfactant flooding in formations containing high salinity water or hard water.	New generation of surfactants, has strong electrolyte tolerance, temperature resistance and thermo stability, better wetting and foaming performance
Dominant Mechanism	Reducing IFT and Wettability Alteration	Reducing IFT	Reducing IFT	Reducing IFT and Wettability Alteration

Figure 4.4.15: Table of the different types of surfactants, their advantages and their mechanism[42]

Type of surfactants

Other scientists [35] have studied the difference between the most common surfactants.

The figure 4.4.15 is a summary of their researches.

IFT stand for interfacial tension and EOR stand for enhanced oil recovery.

The cationic surfactants are group of ions having a positive charge whereas anionic surfactants are group of ions having a negative charge. The nonionic surfactants are species not ionizing in aqueous solutions. They contain two distinct groups: hydrophilic and hydrophobic[42]. The hydrophilic groups include oxyethylene, hydroxyl, carboxyl or amine groups. The hydrophobic group includes alkyls, alkylphenols, or oxypropylenes groups. The zwitterionic surfactants are branched hydrocarbon chains surfactants which compounds a positively charged ion at one end and a negatively charged ion at the other.

Heating treatment

Heating the water-in-oil emulsion is a well way to break the armor envelope of water droplets. It can be use instead of using chemical demulsifiers or electrostatic coalescer which can add significant cost [38] . However, heating the whole emulsion with classical techniques requires a significant amount of energy.

Microwave heating consists in selectively heating the water phase in the emulsion. As a result, the heating cost is reduced. Microwave heating is volumetric, so the entire dispersed water phase is heated instantaneously [37] , on contrary to conventional heating which uses conductive and convective heat transfer. Therefore, the armor envelope of the drops can be destroy.
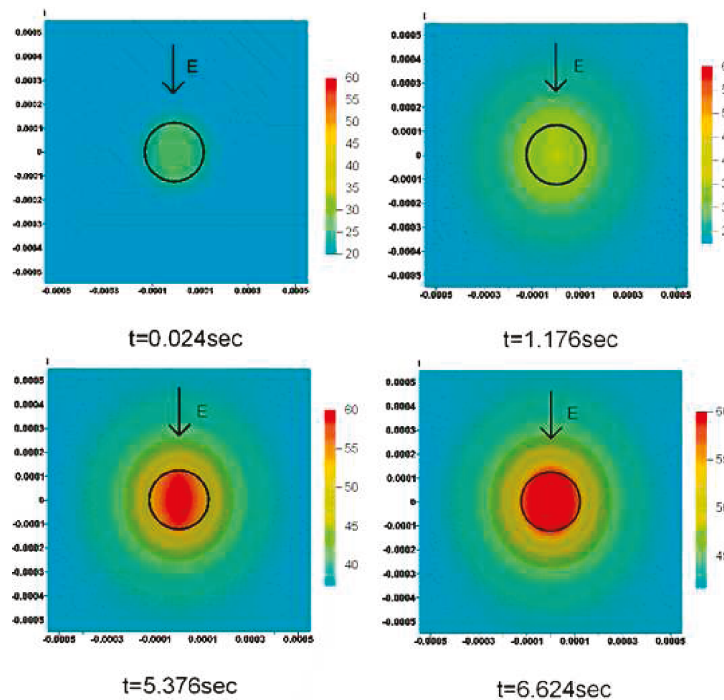

Figure 4.4.16: Simulation of the effect of Microwave radiation on a drop of water during the time[37]

Figure 4.4.16 shows the effects of microwave radiation on a drop of water during the time. We can see that the water is uniformly and quickly heated.

Moreover, microwave heating reduces the viscosity of the oil continuous phase which enhances the water coalsescence.

A study[40] on microwave effects have proved that the optimal range of frequencies to break the armor envelope droplet is approximately 10 GHz. In the same study, the scientists have compared the effects between Radiofrequency field and microwave field on emulsions made of oil in which they added water.

First, they observed the water droplets in samples treated by radiofrequency heating (Figure 4.4.17) and by microwave heating (Figure 4.4.18) . We can see that both heating enhances water coalescence.
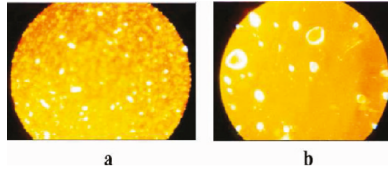

Figure 4.4.17: Picture of a microstructure of an emulsion before the Radiofrequency field effect (a) and after (b)[40]
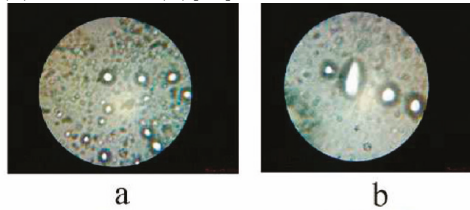

Figure 4.4.18: Picture of the microstructure of an emulsion before the Microwave field effect (a) and after (b)[40]

To quantify the effects of these two methods, they treated an emulsion with various kind of exposure and reported the results in a graph (Figure 4.4.19). The exposures are: radiofrequency heating (red line 1), microwave heating (blue line 2) and conventional calorific heating (green line 3).
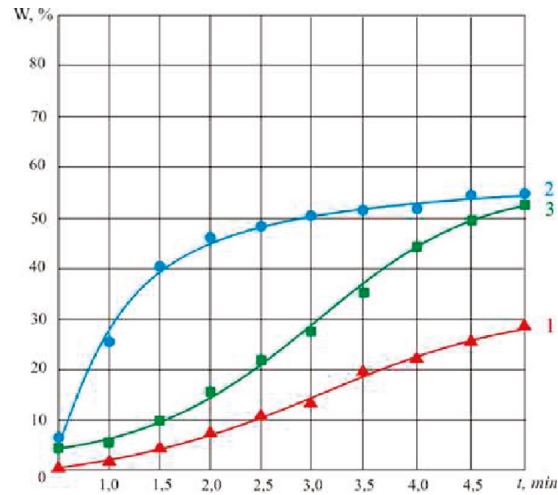
Figure 4.4.19: Graph showing the values of water extracted for different volume proportions of water added into the oil[40]

The percent of water obtained after treatment in relation to the amount of water added in the oil is plotted against the time. We see on this graph that microwave heating treatment is more efficient than radiofrequency heating or conventional heating.

Membrane separation and pH adjustment

A group of scientists have created a new nanostructured mesh film made of copper for separating both water-in-oil and oil-in-water emulsions. [39]
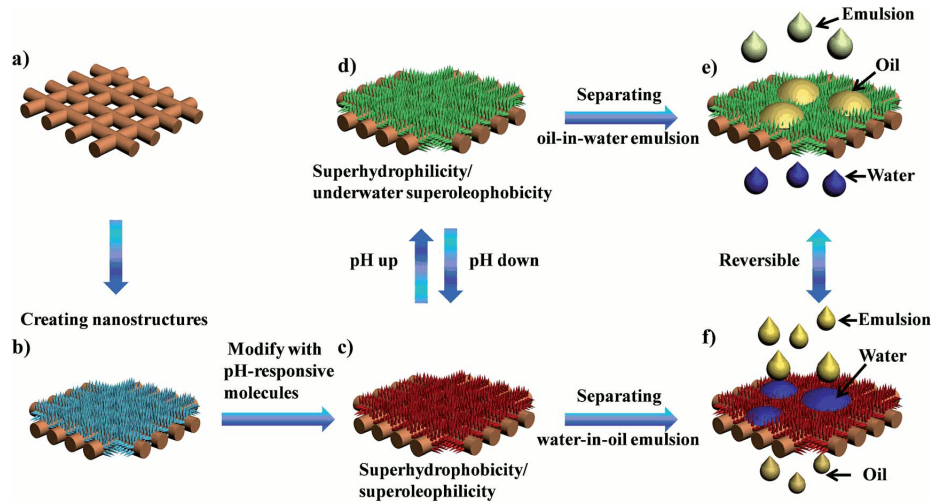
Figure 4.4.20: Design principle for the pH-responsive separating film.[39]

Figure 4.4.20 shows the process of creating the nanostructured mesh film (a-b) and then the process of separation according to the modification of the pH. Whether the pH is raised or dropped, the film becomes either hydrophilic/oleophobic (Figue 8 c-f) to separate oil from oil-in-water emulsions or hydrophobic/oleophilic (Figure 8 d-e) to separate water from water-in-oil emulsions.

Fabrication of the copper mesh film :   The first step is to fabric the nanostructured copper mesh film. A copper mesh substrate is place into a water solution containing $NaOH$ and $(NH_4)_2S_2O_8$. Then, the substrate is dried under N_2 . The second step consists in modifying the substrate with responsive thiol molecules. The substrate of copper is coated with a layer of Au and immersed into an ethanol solution containing $HS(CH_2)_9CH_3$ and $HS(CH_2)_{10}COOH$. Finally, the substrate $Cu(OH)_2$ nanowires is created and dried with N_2 . Figure 4.4.21 shows the structure of the nanowires before (a) and after adding the responsive thiols molecules (b-d). We can see capillaries on the film, they corresponds to the $COOH$ part of thiols molecules added.
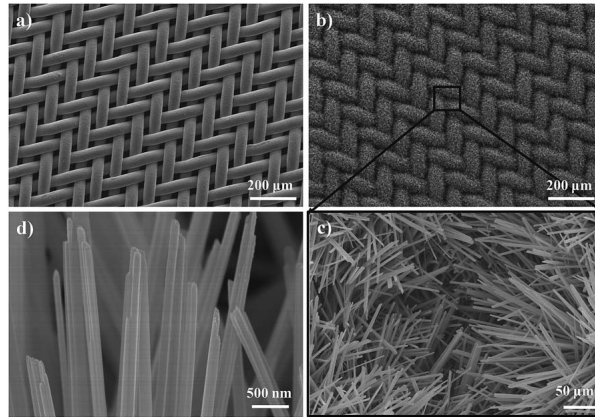
Figure 4.4.21: Images of the copper film substrates: (a) the original substrate, (b-d) after production of $Cu(OH)_2$ nanowires.[39]

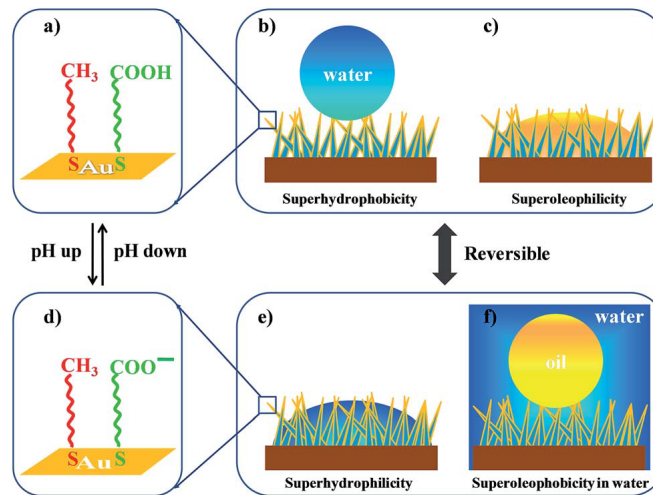**Mechanism of the capillaries:**

Figure 4.4.22: Schematic illustration of the wetting states of the film and the transition process.[39]

Figure 4.4.22 shows the effects of the pH adjustment on the capillaries. On one hand, if the pH is lower than 7 (a), the emulsion is acidic, there are a lot of H^+ and the $COOH$ group is protonated. As a result, the film becomes hydrophobic (b) and do not create bonds with water droplets. In fact, Hydrogen in water forms hydrogen bonds with other molecules. The film becomes

oleophilic (c) and the capillaries allows oil drops to pass through the film. On the other hand, if the pH is higher than 7 (d), the emulsion is basic, they are a lot of OH^- and the $COOH$ group is deprotonated. As a result, hydrogen bonds can be created between the $COOH^-$ groups and the H_2O molecules. The film becomes hydrophilic (e) and allows water drops to pass through the film. It becomes oleophobic (f) and holds the oil drops.

To conclude, the pH adjustment protonate or deprotonate the $COOH$ groups which permit either separating water from water-in-oil emulsions or oil from oil-in-water emulsions.

Efficiency of the separation: Figure 4.4.23 shows the efficiency of the separation for both water-in-oil and oil-in-water emulsion. Before the separation, we can see one opaque phase for the two emulsions. Both of water droplets and oil droplets are discernible. After the separation, we can observe two distinct phases for both emulsions. There are no droplets anymore.

To conclude, we can say that both of water-in-oil and oil-in-water emulsions are well separated using the nanostructured copper mesh film.
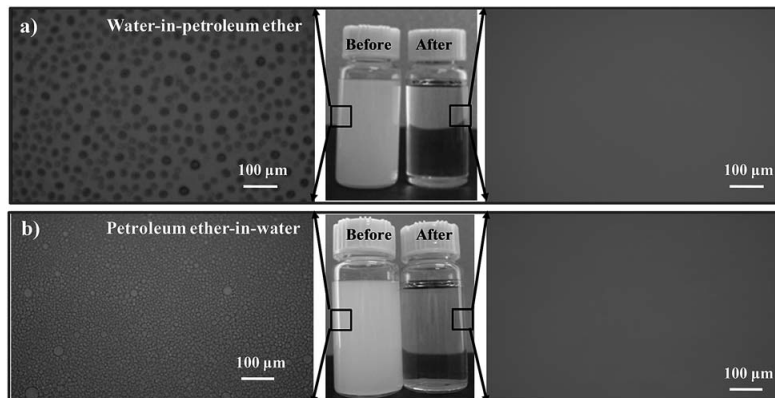

Figure 4.4.23: Photographs of emulsions before and after separation.[39]

E / Presentation of Gerris

Gerris is a Partial Differential Equations Solver (PDES) for the time-dependent incompressible variable-density Euler, Stokes or Navier-Stokes equations (and some variants). Gerris solves the Navier–Stokes equations in 2 or 3 dimensions, allowing to model industrial fluids (aerodynamics, internal flows, etc.) or for instance, the mechanics of droplets, thanks to an accurate formulation of multiphase flows (including surface tension). Most equation solvers use meshes which are either structured (cartesian or curvilinear grids) or unstructured (triangular, tetrahedral, etc). Gerris is quite different on this aspect: it combines structured and unstructured meshes by using a tree data structure, allowing the user to re-

fine locally and dynamically the description of the pressure and velocity fields. Indeed the grid evolves in the course of a given simulation owing to criteria defined by the user (for example, the forces applied to the fluid).

In order to explain how the Gerris language works, we will give the following example which shows the simplest code that can be written with Gerris:

```
1 0 GfsSimulation GfsBox GfsGEdge {} {
        Refine 5
        /*Code Gerris here*/
        OutputSimulation { step = 1 } stdout
}
GfsBox {
        /*Boundary conditions here*/
}
```

Gerris uses a box of length L=1 (in 2D) or a cube (in 3D) to build a domain, in this case we use the 2D solver. "1 0" says one box (1) not connected (0) and the other words (GfsSimulation GfsBox GfsGEdge) are Gerris reserved words. The line "Refine 5" gives us the initial mesh , and it means that Gerris has created a regular cartesian grid with $2^5 = 32$ cells in each dimension. We can use this Gerris keyword to refine the initial mesh. The following figure (Figure 4.4.24) will help us see the impact of the mesh on the resolution of our box:
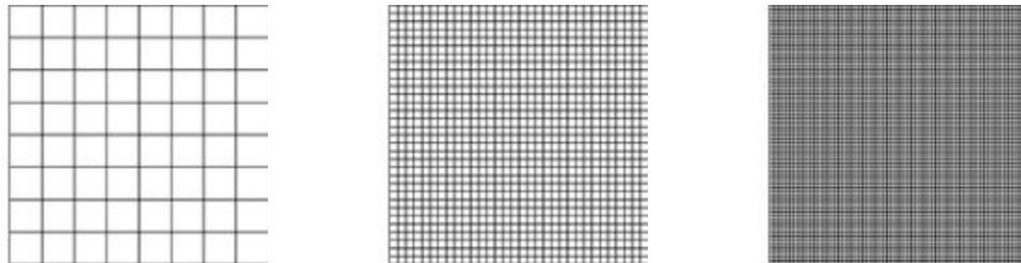

Figure 4.4.24: Resolution. From left to right : Refine 3, Refine 5, Refine 6

Finally, "GFsBox { # boundary conditions here }" allows the user to impose the Boundary conditions for our box. By default Gerris assumes that boundaries are solid walls with slip conditions for the velocity.

Setting the different conditions in Gerris: Gerris uses two families of words: "GfsBoundary" and "GfsBc", with the corresponding inheritances. **Gfs-Boundary** is used to define boundary conditions on the boundaries for the box with the following syntax:

```
GfsBoundary {
        [ GfsBc ]
        [ GfsBc ]
```

```
}
```

« GfsBc » allows the user to change the following parameters:

- GfsBcDirichlet — Dirichlet boundary condition (i.e. value of the velocity U, the volume V and the pressure P)

- GfsBcNeumann — Neumann boundary condition (i.e. value of the normal derivative)

- GfsBcNavier — Navier slip/Robin boundary condition

- GfsBoundaryInflowConstant — Constant inflow

- GfsBoundaryOutflow — Free outflow/inflow

For example, we can set the pressure as 1 at the left, 0 at the right, a sinusoidal velocity at the top and an outflow condition on the bottom using this piece of code:

```
GfsBox {
        left = Boundary {
                BcDirichlet P 1
                }
        right = Boundary {
                BcDirichlet P 0
                }
        top = Boundary {
                BcDirichlet U ( sin(2.*M_PI*0.05*t) )
                        }
        Bottom = BoundaryOutflow
}
```

The Gerris word **GfsTime** defines the physical and the computational time (number of steps performed). By default both the physical time and the time step number are zero when the program starts. It is possible to set different values using for example :

```
GfsTime { t = 1.4 i = 32 }
```

where **i** is the time step number and **t** is the physical time. The end identifier specifies that the simulation should stop when the physical time reaches the given value. It is also possible to stop the simulation when a specified number of time steps is reached, using the iend identifier. If both end and iend are specified, the simulation stops when either of these is reached. By default, both end and iend values are infinite.

```
GfsTime { end = 2 iend = 32 }
```

Gerris allows us to also change the viscosity of the fluid using the function **GfsSourceViscosity**. The viscosity is zero by default.

Gerris can also model the physical characteristics of the frontier, Gerris uses two reserved words:

- **GfsSourceTension** which adds a surface-tension term to the momentum equations, associated with an interface defined by its volume fraction and curvature. The syntax radiusused is: **GfsSourceTension** tracer value-of-tension variable-of-curvature

- **GfsVariableCurvature** which contains the mean curvature (double the mean curvature in 3D) of an interface. The syntax used is: **GfsVariable-Curvature** variable-of-curvature tracer

For example, to add a surface tension to a bubble we set :

```
VariableCurvature K T1
SourceTension T1 0.1 K
```

Adding objects to the simulation: In order to add a solid object in our simulation file, Gerris uses implicit functions to define solids, the Gerris keyword is **GfsSolid** and the syntax is :

```
GfsSolid ( implicit function )
```

For example, a circle of radius 0.125 at (0,0) will be written in the code like this :

```
Solid (x*x + y*y - 0.125*0.125)
```

We can also refine the solid using the Gerris keyword **RefineSolid**.

Visualization of the Gerris file: In order to visualize the Gerris simulation files, we can use GfsView which is a tool written especially for this purpose. We use the following syntax:

```
gfsview2D file.gfs
```

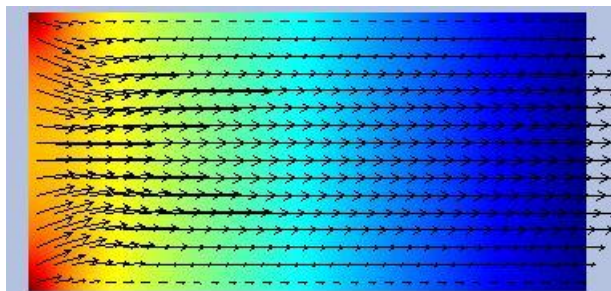The result will look like the following figure 4.4.25:

Figure 4.4.25: Flow simulation using Gerris

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